Topics in Non-perturbative Quantum Field Theory

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Abstract

Axiomatic formulations of quantum field theory (QFT) provide a powerful framework from which non-perturbative questions can be addressed. In this thesis, these formulations are applied and developed in order to shine new light on a variety of different unresolved problems in particle physics. One such problem is the spin structure of hadrons, a topic which despite intense theoretical investigation still remains poorly understood. We propose a new approach to this problem that emphasises the importance of dealing with spatial boundary operators in a rigorous manner. Adopting this approach, it appears that the spin of a hadron is not simply determined by the spin of its constituents, and that in fact such a decomposition is prohibited by the non-perturbative structure of quantum chromodynamics (QCD). The next problem investigated concerns the behaviour of correlation functions, and how one can obtain information about the non-perturbative properties of these objects. To do so, we develop a non-perturbative procedure which exploits the general structural relations satisfied by correlation functions. By applying this procedure to specific correlators in scalar field theory and QCD, it is shown that novel constraints are imposed both on the spectral densities of these correlators and the condensates in these theories. As is the case with the structure of hadronic spin, spatial boundary operators also play an important role in the quantisation of non-manifest symmetries. We explicitly demonstrate that the potential non-vanishing of this class of operators implies that the charge generator of the symmetry is non-unique, unless one knows how the charge operator acts on the vacuum state. For Poincaré symmetry the uniqueness of the vacuum fixes the corresponding charges, whereas for supersymmetry there exists no such physical requirement, which suggests that the action of the supersymmetric charge on states is potentially ambiguous. The thesis is concluded with an investigation into confinement in QCD. More specifically, by analysing the asymptotic structure of cluster correlators, we derive a condition on the correlation strength between clusters of fields at large distances. It turns out that if the correlation strength between clusters of coloured fields increases when the distance between the clusters is increased, this is sufficient to imply confinement. By applying our derived condition, we conclude that certain lattice QCD calculations of the quark and gluon propagators suggest that quarks and gluons are in fact confined in this manner.

This thesis is based on the work in Refs. [1–4].

Zusammenfassung

Axiomatische Formulierungen von Quantenfeldtheorien (QFT) bilden ein vielseitiges Wekzeug, welches es uns erlaubt Fragestellungen nichtperturbativer Probleme zu bearbeiten. In der vorliegenden Dissertation werden axiomatische Formulierungen entwickelt, und auf verschiedene Probleme im Bereich der Teilchenphysik angewendet. Eines dieser Probleme umfasst die Spinstruktur von Hadronen. Trotz langjähriger theoretischer Untersuchungen ist diese weiterhin nur hinreichend verstanden. Wir schlagen hier einen neuen Zugang zu dieser Thematik vor, in welchem wir insbesonders die Wichtigkeit des mathematisch korrekten Umganges mit dem Operator der räumlichen Randbedingungen beim Angehen dieses Problems hervorheben. Mit unserem Ansatz können wir zeigen, dass der hadronische Spin sich nicht, wie bisher angenommen, einfach in die Spins seiner Konstituenten zerlegen lässt. In der Tat zeigen wir, dass dieser Ansatz der Zerlegeung generell aufgrund der nichtperturbativen Natur der Quantenchromodynamik (QCD) unmöglich ist. Im Weiteren beschäftigen wir uns mit dem Verhalten von Korrelationsfunktionen, und untersuchen die Möglichkeit Informationen über die nichtperturbativen Eigenschaften dieser Objekte zu inferieren. Die Anwendung dieses Ansatzes auf die spezifischen Korrelatoren, welche in skalaren Feldtheorien und QCD auftreten, liefert neuartige Beschränkungen der Spektraldichten und Kondensate dieser Theorien. Wie auch im Fall des hadronischen Spins spielen auch hier die Operatoren für die räumlichen Grenzen ein wichtige Role in der Quantisierung nichtmanifester Symmetrien. Wir zeigen explizit, dass diese Operatorklassen möglicherweise nicht vernachlässigbar sind, welches eine nicht mehr eindeutige Definition des Ladungsgenerators impliziert, solange der Ladungsgenerator nicht auf den Vakuumszustand angewendet wird. Im Falle der Poincaré-Symmetrie sind die entsprechenden Ladungen durch die Einzigartigkeit des Vacuums festgelegt. wohingegen in Supersymmetrie keine

solche physikalische Bedingung existiert. Dies suggeriert, dass die Wirkung der supersymmetrischen Ladung auf Zustände potentiell mehrdeutig ist. Zum Abschluss dieser Dissertation leiten wir eine Bedingung für die Korrelationsstärke zwischen Feldclustern über große Abständer her. Dabei zeigt sich, dass ein Anwachsen der Korrelationsstärke zwischen Clustern farbgeladener Felder bei wachsenden Abstand zwischen den Feldern ausreicht, um Confinement zu implizieren. Die Anwendung der hier hergeleiteten Bedingung lässt uns basierend auf Lattice QCD Berechnungen der Quark- und Gluonpropagatoren schlussfolgern, dass Quarks und Gluonen in der Tat auf diese Weise confined sind.

Diese Dissertation basiert auf den Referenzen [1–4].

Contents

Chapter 1

Introduction

1.1 Particle physics at a crossroads

Particle physics is currently at a crossroads. The Standard Model (SM) of particle physics, which was mostly developed during the 1960s [5–9] and 1970s [10, 11] to provide a unified description of the strong, weak and electromagnetic interactions has, over the last few decades, been verified to extraordinary precision [12]. The recent discovery of the Higgs boson at the ATLAS and CMS experiments at CERN [13, 14] marks the verification of the final major untested prediction of this hugely successful theory. However, it is clear that the SM cannot be the full picture, the most obvious reason being that it does not include the interactions associated with gravity. Moreover, the existence of dark matter [15], dark energy [16], and significant baryon asymmetry [17], all lack an explanation within the SM. Many theoretical explanations have been put forth to try and understand these features, most of which involve modifying or expanding the SM theory itself [18].

Perhaps the most prominent proposed beyond the SM (BSM) theory is supersymmetry[1]. Supersymmetry corresponds to an enlargement of the Poincaré group of spacetime

[1] A detailed overview of the properties and characteristics of supersymmetry can be found in [19] and [20].

symmetries via the inclusion of additional internal symmetries, which are generated by spinor-valued charges. The fact that the supersymmetric charges are fermionic enables the theory to evade the famous *Coleman-Mandula theorem* [21], which states the impossibility of combining internal and spacetime symmetries in a non-trivial manner. An important consequence of supersymmetry is that the extended symmetry operators map fermionic and bosonic states to one another, which means that for every known particle there must exist a corresponding *superpartner* particle. This feature in particular has been proposed as a solution to the dark matter problem, since many supersymmetric models contain dark matter candidates. Another prominent class of BSM models are Technicolor theories. These theories are strongly interacting models that aim to explain electroweak symmetry breaking via a dynamical mechanism [22, 23]. The major advantage of Technicolor is that the parameters associated with this mechanism, such as the electroweak scale, arise automatically from the theory in much the same way that the scale Λ_{QCD} does in the theory of strong interactions, quantum chromodynamics (QCD) [24]. Much like supersymmetric models, the particle content of Technicolor theories are not fully constrained by the symmetries of the theories themselves, and so a large variety of different models are possible [25]. Besides supersymmetry and Technicolor, there are many other proposed BSM theories including loop quantum gravity [26], theories of extra dimensions [27], and string theory [28], but these will not be discussed further here.

Many proposed BSM theories are now being directly tested in different experiments all over the world, with some of the most stringent tests being performed at the Large Hadron Collider (LHC) at CERN. Although a few deviations have been observed [29–31], recent results are now starting to cast doubt on several of these proposed BSM theories [32–35]. The LHC will continue to run over the next few years and provide considerably more data, which may well reveal interesting new features. However, so far no significant deviations to the SM, which are unambiguously describable by a specific BSM theory, have yet been observed. This poses an important question: *why have BSM theories been so unsuccessful?* Of course, one reason may be that some of these models are in fact correct, but are only observable at energies beyond the range of the LHC. In order to incorporate current SM predictions into these BSM theories though, this usually requires a certain degree of fine-tuning of the model parameters [36]. The lack of success of BSM theories demonstrates that the SM has withstood significant experimental scrutiny. Nevertheless, many features of the SM itself are still poorly understood. In QCD, a prominent such example is the non-observation of quarks and gluons in experiments [37–39]. This has led to the hypothesis of the existence of a *confinement mechanism*, which acts to prevent these states from being observed [40]. Even though this mechanism is implicitly assumed in many applications of QCD, its precise nature, and in fact its very existence, remain open questions. Similarly, the connection between the physics of hadrons and QCD is a feature which is widely accepted, but remains largely unknown. In other words, it is still not fully clear how to describe the dynamics and properties of hadrons using QCD. In order to have any chance of fully understanding SM features such as these, as well as establishing why BSM models have so far been unsuccessful, it is imperative that these theories are analysed with a significant degree of theoretical scrutiny. Not only might this help answer these questions, but it may also provide important clues for future theoretical directions.

1.2 Axiomatic approaches to quantum field theory

1.2.1 Motivations

From a theoretical perspective, perturbation theory has proven to be an extremely successful approach for checking the internal consistency of quantum field theories (QFTs) [41–45]. Nevertheless, perturbation theory is, by its very construction, only valid in a weakly interacting regime, and so cannot possibly provide a full description of a quantised theory. An illustrative example of this deficiency is the divergence of perturbative series, which was first argued for QED by Dyson [46]. This argument considers some renormalised physical quantity $F(e^2)$, which has the following perturbative expansion (around $e^2 = 0$):

$$F(e^2) = F(0) + F_2(0)e^2 + F_4(0)e^4 + \cdots$$

If this series were convergent then this would imply that $F(e^2)$ is analytic in some neighbourhood of $e^2 = 0$, and hence $F(-e^2)$ is *also* a well-defined analytic function, with a convergent power series expansion in this neighbourhood. The fact that opposite charges attract one another in QED implies that the energy of the system must have a lower bound. This follows from the observation that if one brings groups of oppositely charged particles close together, inevitably this implies that charged particles of equal sign will *also* become close together, and will create repulsive forces that prevent the potential energy of the system from being lowered indefinitely. However, $F(-e^2)$ corresponds to the value of F in a theory in which like charges attract, since the Coulomb force law changes sign when $e^2 \to -e^2$. This means that one can group together particles with charges of the same sign without inducing any repulsive forces, and hence the energy of the system can be indefinitely lowered. Since the vacuum state is no longer the lowest energy state, it follows that the theory must be unstable, and hence QED has opposite stability properties in the regimes above and below $e^2 = 0$. If the physical quantity $F(e^2)$ were analytic, this would imply that $F(e^2)$ varies smoothly under the transition $e^2 \to -e^2$. But clearly this contradicts the discontinuity between the two regimes, and so one can conclude that the perturbative expansion of $F(e^2)$ must diverge [46]. Although it is difficult to establish whether a specific perturbative series diverges or not, Dyson's conclusion has been proved to be correct in several simple (low-dimensional) QFT models [47]. The fact that perturbative series appear to be divergent suggests that perturbation theory cannot be sufficient for fully describing the structure of a QFT.

Another issue that arises from using a purely perturbative approach is connected to the following important theorem [48, 49]:

Theorem (Haag)**.** *Assume* $\{\varphi_1\}$ *and* $\{\varphi_2\}$ *are the fields of QFTs with vacuum states* $|0\rangle_1$ *and* $|0\rangle_2$ *respectively. If the fields are connected by some unitary transformation* V*, this implies that:* $V|0\rangle_1 = c|0\rangle_2$*, where* $c \in \mathbb{C}$ *has modulus one.*

An immediate consequence of *Haag's Theorem* is that if one of the two QFTs defines a free theory, then the other must *also* define a free theory. This conclusion is particularly relevant for the interaction picture approach to scattering theory, where (Heisenberg) operators $A_H(t)$ evolving under the full Hamiltonian H are connected to interaction (or Dirac) picture operators $A_I(t)$, evolving under the free Hamiltonian $H_0 := H - gH_I$, via the hypothesised relation [50]:

$$A_I(t) = U(t)A_H(t)U(t)^{-1}$$

with $U(t)$ a unitary operator. By defining $U(t_2, t_1) := U(t_2)U(t_1)^{-1}$, it follows that $U(t_2, t_1)$ is calculable using the integral equation:

$$U(t_2, t_1) = \mathbb{I} - i\int_{t_1}^{t_2} ds\ gH_I(s)U(s, t_1)$$

where $H_I(s)$ is a functional of the (free) interaction picture fields. Assuming that the coupling constant g is small, a perturbative approximation to $U(t_2, t_1)$ can then be calculated (recursively) up to some order in g. The scattering matrix S is then defined by: $S := \lim_{t\to\infty, t'\to-\infty} U(t, t')$. The (perturbative) calculation of S is essential for the determination of scattering amplitudes, and hence measurable quantities such as cross-sections. However, because of Haag's Theorem it follows that if the operator $U(t)$ exists and $A_I(t)$ does indeed evolve under the free Hamiltonian H_0, then $A_H(t)$ must *also* evolve under H_0 and not H. In particular, the (Fock space) ground state $|0\rangle_{\mathrm{F}}$ of the free Hamiltonian H_0 must coincide with the ground state $|0\rangle$ of H, and this is only valid if $g = 0$. The existence of $U(t)$ is therefore not compatible with the free evolution of $A_I(t)$, and so *the interaction picture cannot exist.* This striking conclusion undermines the assumption that perturbation theory alone is sufficient for understanding scattering processes in QFT, and highlights the need for a non-perturbative approach[2].

The lack of convergence of perturbative series and Haag's Theorem are results which both demonstrate that a non-perturbative approach is essential if one is to fully understand the subtleties of QFT. An important example of such an approach is axiomatic QFT (AQFT). This approach consists of defining a QFT in a mathematically rigorous manner via the definition of a series of physically motivated axioms [47, 49–52]. Since these axioms are hypothesised to hold in general, independently of the regime to which the theory is applied, AQFT defines a powerful framework from which both perturbative and non-perturbative phenomena can be rigorously understood[3]. In the next two sections a general overview of AQFT will be given (Sec. 1.2.2), and some prominent consequences of AQFT will be discussed (Sec. 1.2.3).

1.2.2 The Wightman axioms

Although there are several different axiomatic formulations of QFT, generally these formulations contain the following core set of axioms which are often referred to as the *Wightman axioms* [47, 49, 50, 56]:

Axiom 1 (**Hilbert space structure**). *The states of the theory are rays in a Hilbert space $\mathcal{H}$ which possesses a continuous unitary representation $U(a,\alpha)$ of the Poincaré spinor group $\overline{\mathscr{P}_{+}^{\uparrow}}$.*

Axiom 2 (**Spectral condition**). *The spectrum of the energy-momentum operator*

[2]One can in fact rigorously define an S-matrix S_H in a non-perturbative manner without reference to the interaction picture or perturbation theory [50]. The corresponding Heisenberg picture operator S_H is defined by: $\langle\Psi_{\beta}^{+}|\Psi_{\alpha}^{-}\rangle = \langle\Psi_{\beta}^{+}|S_H|\Psi_{\alpha}^{+}\rangle$, where $|\Psi_{\alpha}^{-}\rangle$ and $|\Psi_{\beta}^{+}\rangle$ are asymptotic *in* and *out* states respectively [50]. Under certain conditions, the construction of S_H is actually equivalent to the construction of S. The violation of these conditions is connected to the appearance of infrared divergences in the perturbative expansion of S [47].

[3]Although both perturbative and non-perturbative quantities can be well-defined using AQFT, the actual calculation of non-perturbative quantities is generally more involved. Lattice quantum field theory (LQFT), which is constructed by discretising QFTs on a spacetime lattice, provides one such way in which these quantities can be computed [53–55].

P^μ is confined to the closed forward light cone $\overline{V}^+ = \{p^\mu \mid p^2 \geq 0,\, p^0 \geq 0\}$, where $U(a,1) = e^{iP^\mu a_\mu}$.

Axiom 3 (**Uniqueness of the vacuum**). *There exists a unit state vector $|0\rangle$ (the vacuum state) which is a unique translationally invariant state in $\mathcal{H}$.*

Axiom 4 (**Field operators**). *The theory consists of fields $\varphi^{(\kappa)}(x)$ (of type (κ)) which have components $\varphi_l^{(\kappa)}(x)$ that are operator-valued tempered distributions in $\mathcal{H}$, and the vacuum state $|0\rangle$ is a cyclic vector for the fields.*

Axiom 5 (**Relativistic covariance**). *The fields $\varphi_l^{(\kappa)}(x)$ transform covariantly under the action of $\overline{\mathscr{P}_+^\uparrow}$:*

$$U(a,\alpha)\varphi_i^{(\kappa)}(x)U(a,\alpha)^{-1} = S_{ij}^{(\kappa)}(\alpha^{-1})\varphi_j^{(\kappa)}(\Lambda(\alpha)x + a)$$

where $S(\alpha)$ is a finite dimensional matrix representation of the Lorentz spinor group $\overline{\mathscr{L}_+^\uparrow}$, and $\Lambda(\alpha)$ is the Lorentz transformation corresponding to $\alpha \in \overline{\mathscr{L}_+^\uparrow}$.

Axiom 6 (**Local (anti-)commutativity**). *If the support of the test functions f, g of the fields $\varphi_l^{(\kappa)}, \varphi_m^{(\kappa')}$ are space-like separated, then:*

$$[\varphi_l^{(\kappa)}(f), \varphi_m^{(\kappa')}(g)]_\pm = \varphi_l^{(\kappa)}(f)\varphi_m^{(\kappa')}(g) \pm \varphi_m^{(\kappa')}(g)\varphi_l^{(\kappa)}(f) = 0$$

when applied to any state in $\mathcal{H}$, for any fields $\varphi_l^{(\kappa)}, \varphi_m^{(\kappa')}$. In particular, $\varphi_l^{(\kappa)}(f)\varphi_m^{(\kappa')}(g) = \sigma^{(\kappa,\kappa')}\varphi_m^{(\kappa')}(g)\varphi_l^{(\kappa)}(f)$, where $\sigma^{(\kappa,\kappa')} = 1$ if at least one of the fields has integer spin and $\sigma^{(\kappa,\kappa')} = -1$ if both fields have half-integer spin.

Axioms 1–4 largely describe the quantum mechanical structure of a QFT. In Axiom 1 the existence of a unitary representation of $\overline{\mathscr{P}_+^\uparrow}$ physically corresponds to the requirement that the theory is invariant under (orientation and time preserving) Poincaré transformations. In fact, it follows from *Wigner's Theorem*[4] that the Poincaré invariance of a quantum theory implies the existence of a unitary representation $U(a,\alpha)$ of $\overline{\mathscr{P}_+^\uparrow}$, which describes the effect of Poincaré transformations on the states in $\mathcal{H}$. The group $\overline{\mathscr{P}_+^\uparrow}$ is the universal cover of the restricted Poincaré group $\mathscr{P}_+^\uparrow = \mathbb{R}^{1,3} \rtimes \mathscr{L}_+^\uparrow$, where $\mathscr{L}_+^\uparrow \cong \mathrm{SO}^+(1,3)$ is the identity component of the full Lorentz group[5] $\mathscr{L}$, and

[4]See [50] for more details.

[5]The full Lorentz group $\mathscr{L} \cong \mathrm{O}(1,3)$ has four connected components: $\mathscr{L}_+^\uparrow$, $\mathscr{L}_-^\uparrow$, $\mathscr{L}_+^\downarrow$ and $\mathscr{L}_-^\downarrow$ [49].

consists of Lorentz transformations which preserve both orientation and the direction of time[6]. The reason why the Poincaré subgroup $\mathscr{P}_+^\uparrow$ is used instead of $\mathscr{P}$ is that the full group[7] contains parity and time-reversal transformations, which are known to not always be physically preserved. An important example of this is in the theory of weak interactions, where parity is violated [57–59]. Another interesting feature of Axiom 1 is that U is a representation of the universal cover of the restricted Poincaré group $\overline{\mathscr{P}_+^\uparrow}$, as opposed to $\mathscr{P}_+^\uparrow$ itself. This feature originates from the fact that states are defined by *rays* of the Hilbert space, which are equivalence classes $[|\Psi\rangle]$ of vectors in $\mathcal{H}$ where: $|\Phi\rangle \in [|\Psi\rangle]$ if $|\Phi\rangle = \lambda|\Psi\rangle$ for some $\lambda \in \mathbb{C}$. So two vectors correspond to the same state if they differ by a multiplication of a complex number. This means that Poincaré invariance actually implies the existence of transformations $\overline{U}$ which act on the space of rays[8] and not $\mathcal{H}$ itself, and so the induced transformations U on $\mathcal{H}$ are only determined up to an arbitrary phase factor $e^{i\phi}$, i.e. U defines a *projective representation* of $\mathscr{P}_+^\uparrow$ [50]. In order to guarantee that each transformation $U(a,\alpha)$ is unambiguously specified, it is natural to extend the map U to the covering group $\overline{\mathscr{P}_+^\uparrow}$, since this ensures that U is an ordinary representation [50]. The physical consequence of this is that $\mathcal{H}$ is able to contain fermionic states, because unlike $\mathscr{P}_+^\uparrow$, $\overline{\mathscr{P}_+^\uparrow}$ permits spinor representations.

The physical motivation behind the spectral condition (Axiom 2) is that it ensures that the Hamiltonian is bounded from below, which is necessary to guarantee the stability of the theory [47]. Axiom 3 demands that there exists a state $|0\rangle$ (the vacuum) which is both unique and invariant under spacetime translations ($U(a,1)|0\rangle = |0\rangle$). Due to the Poincaré group law structure, together these properties are sufficient to imply: $U(0,\alpha)|0\rangle = |0\rangle$, and that $|0\rangle$ is therefore invariant under all (orientation and time preserving) Poincaré transformations [47]. Physically speaking this means that the vacuum state looks the same to all observers [49]. Axiom 4 is of central importance in the definition of QFTs because it defines a key characteristic of quantised fields $\varphi_l^{(\kappa)}(x)$ – they are *operator-valued distributions*. Although there are several technical reasons for why quantised fields are distributions as opposed to function[9], the physical motivation

[6]Sometimes $\overline{\mathscr{P}_+^\uparrow} = \mathbb{R}^{1,3} \rtimes \overline{\mathscr{L}_+^\uparrow}$ is referred to as the *Poincaré spinor group* because $\overline{\mathscr{L}_+^\uparrow} \cong \mathrm{SL}(2,\mathbb{C})$ is isomorphic to the spin group $\mathrm{Spin}^+(1,3)$, which has spinor representations.

[7]The full Poincaré group has the structure: $\mathscr{P} = \mathbb{R}^{1,3} \rtimes \mathscr{L}$.

[8]The space of rays of $\mathcal{H}$ is the projective Hilbert space $P(\mathcal{H})$.

[9]See [47, 49, 50, 60] for a more in-depth discussion of this issue.

arises from the fact that operators inherently imply a measurement, so if a field $\varphi_l^{(\kappa)}(x)$ *were* a well-defined operator then this would represent the performance of a measurement at a single spacetime point x. But this is ruled out quantum mechanically since this would require an infinite amount of energy [50]. Instead, the distributional behaviour of quantised fields $\varphi_l^{(\kappa)}$ implies that they must be smeared with an appropriate test function f in order to define a convergent operator $\varphi_l^{(\kappa)}(f) := \int d^4x \ \varphi_l^{(\kappa)}(x)f(x)$. If the test function has support in some spacetime region $\mathcal{U} \subset \mathbb{R}^{1,3}$, then the action of $\varphi_l^{(\kappa)}(f)$ on a state corresponds to the performance of a measurement in $\mathcal{U}$. Fields $\varphi_l^{(\kappa)}$ are in particular assumed to be tempered distributions ($\varphi_l^{(\kappa)} \in \mathcal{S}'$) and the test functions f are Schwartz functions $\mathcal{S}$ defined on spacetime[10]. A key feature of tempered distributions is that their Fourier transforms always exist, and that they themselves are also tempered distributions [62]. Physically, this is an important property because it guarantees that the position and momentum space descriptions of a QFT are always compatible. The other requirement from Axiom 4 is that the vacuum state $|0\rangle$ is a cyclic vector for the fields, i.e. the space of states constructed by acting with the field algebra[11] $\mathcal{F}(\mathbb{R}^{1,3})$ on $|0\rangle$, is dense in $\mathcal{H}$ [47]. In essence, this means that the field degrees of freedom are sufficient for characterising all possible states in $\mathcal{H}$, and hence provide a complete physical description of a QFT [49].

In contrast to Axioms 1–4, Axioms 5 and 6 define the relativistic properties of a QFT. Axiom 5 requires that the fields transform in a relativistically covariant manner[12], which is important because this guarantees that the QFT is manifestly covariant [47]. Moreover, the global transformation properties of the field components are the same as those of the irreducible representations of $\overline{\mathscr{P}_+^\uparrow}$ [49, 50], and this provides the connection between the permitted physical states and the field degrees of freedom which define them. The physical motivation for local (anti-)commutativity (Axiom 6) is that it imposes a causality restriction on the theory. This arises because, as previously mentioned, the action of field operators $\varphi_l^{(\kappa)}(f)$ on states corresponds to the performance of a particular measurement in the spacetime region supp(f) [50]. So given that another

[10] See [61, 62] for a discussion of the general properties of distributions, and in particular the spaces $\mathcal{S}'$ and $\mathcal{S}$.

[11] The field algebra $\mathcal{F}(\mathbb{R}^{1,3})$ is the polynomial algebra of fields smeared with test functions in $\mathcal{S}(\mathbb{R}^{1,3})$.

[12] Technically the relativistic covariance condition is defined for smeared fields, and so Axiom 5 should be understood to implicitly involve a smearing with test functions [49].

measurement $\varphi_m^{(\kappa')}(g)$ is performed in a region $\mathrm{supp}(g)$, which is space-like separated to $\mathrm{supp}(f)$, local (anti-)commutativity states that these two measurements must either commute or anti-commute with one another. Physically speaking this means that measurements which are performed a space-like distance apart cannot be causally related to one another. Often local (anti-)commutativity is instead phrased in the following manner[13]: $[\varphi_l^{(\kappa)}(x), \varphi_m^{(\kappa')}(y)]_\pm = 0$ *when* $x - y$ *is space-like, and hence:* $(x-y)^2 < 0$, with the implicit understanding that the fields are actually smeared with test functions as in Axiom 6.

1.2.3 The non-perturbative consequences of the Wightman axioms

The Wightman axioms outlined in Sec. 1.2.2 are central to the proof of many profound results in QFT. Before discussing these results, it is important to first describe the effect that these axioms have on the vacuum expectation values of products of fields[14] $\mathcal{W}_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}(x_1,...,x_n) := \langle 0|\varphi_{l_1}^{(\kappa_1)}(x_1)\cdots\varphi_{l_n}^{(\kappa_n)}(x_n)|0\rangle$, which turn out to be the objects of central importance in any QFT. Due to Axioms 1–6 these objects satisfy the following properties [47, 49, 56]:

P. 1 (**Distributional**). $\mathcal{W}_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}(x_1,...,x_n)$ *is a tempered distribution in* $\mathcal{S}'((\mathbb{R}^{1,3})^n)$.

P. 2 (**Covariance**). *There exist distributions* $W_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)} \in \mathcal{S}'((\mathbb{R}^{1,3})^{n-1})$ *(also called Wightman functions) such that:*

$$\mathcal{W}_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}(x_1,...,x_n) = W_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}(\xi_1,...,\xi_{n-1})$$

where $\xi_i = x_i - x_{i+1}$. *Moreover,* $W_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}$ *satisfies:*

$$S_{l_1 m_1}^{(\kappa_1)}(\alpha^{-1})\cdots S_{l_n m_n}^{(\kappa_n)}(\alpha^{-1}) W_{m_1\cdots m_n}^{(\kappa_1\cdots\kappa_n)}(\Lambda(\alpha)\xi_1,...,\Lambda(\alpha)\xi_{n-1}) = W_{l_1\cdots l_n}^{(\kappa_1\cdots\kappa_n)}(\xi_1,...,\xi_{n-1})$$

for all $\alpha \in \overline{\mathscr{L}_+^\uparrow} \cong \mathrm{SL}(2,\mathbb{C})$.

[13] Both conventions will be used interchangeably throughout this thesis.

[14] In the context of the Wightman axioms, these objects are referred to as *Wightman functions* [47, 50].

P. 3 (**Spectral condition**). *The Fourier transform* $\widehat{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}$ *of* $W^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}$ *has the support property:*

$$supp\ \widehat{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(p_1,...,p_{n-1}) \subset \overline{V}^+ \times \cdots \times \overline{V}^+$$

and hence $\widehat{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(p_1,...,p_{n-1}) = 0$ *if* $p_i \notin \overline{V}^+$ *for some* i.

P. 4 (**Locality**). *One has that:*

$$\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n) = \sigma^{(\kappa_i,\kappa_{i+1})}\mathcal{W}^{(\kappa_1\cdots\kappa_{i-1}\kappa_{i+1}\kappa_i\cdots\kappa_n)}_{l_1\cdots l_{i-1}l_{i+1}l_i\cdots l_n}(x_1,...,x_{i-1},x_{i+1},x_i,...,x_n)$$

when $x_i - x_{i+1}$ *is space-like, i.e.* $(x_i - x_{i+1})^2 < 0$.

P. 5 (**Hermiticity**). *The conjugate of* $\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}$ *satisfies:*

$$\overline{\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n)} = \mathcal{W}^{(\bar\kappa_n\cdots\bar\kappa_1)}_{\bar l_n\cdots\bar l_1}(x_n,...,x_1)$$

where: $\mathcal{W}^{(\bar\kappa_n\cdots\bar\kappa_1)}_{\bar l_n\cdots\bar l_1}(x_n,...,x_1) := \langle 0|(\varphi^{(\kappa_n)}_{l_n})^*(x_n)\cdots(\varphi^{(\kappa_1)}_{l_1})^*(x_1)|0\rangle$

P. 6 (**Positive definiteness**). $\mathcal{W}^{(\bar\kappa_m\cdots\bar\kappa_1\kappa'_1\cdots\kappa'_n)}_{\bar l_m\cdots\bar l_1 l'_1\cdots l'_n}(x_m,...,x_1,x'_1,...,x'_n)$ *satisfies the inequality:*

$$\sum_{n,m=0}^{\infty}\int d^4x_1\cdots d^4x_m\int d^4x'_1\cdots d^4x'_n\ \mathcal{W}^{(\bar\kappa_m\cdots\bar\kappa_1\kappa'_1\cdots\kappa'_n)}_{\bar l_m\cdots\bar l_1 l'_1\cdots l'_n}(x_m,...,x_1,x'_1,...,x'_n)$$
$$\times f^{(\kappa_1\cdots\kappa_m)}_{l_1\cdots l_m}(x_1,...,x_m) f^{(\kappa'_1\cdots\kappa'_n)}_{l'_1\cdots l'_n}(x'_1,...,x'_n) \geq 0$$

where: $\{f^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}\}$ *are any sequence of test functions in* $\mathcal{S}((\mathbb{R}^{1,3})^n)$ *where only a finite number of* $f^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}$ *are non-zero, and* $f^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}$ *is an arbitrary complex number for* $n = 0$.

P. 7 (**Cluster**). *For any space-like vector* $a \in \mathbb{R}^{1,3}$

$$\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_i,x_{i+1}+\lambda a,...,x_n+\lambda a)\ \to\ \mathcal{W}^{(\kappa_1\cdots\kappa_i)}_{l_1\cdots l_i}(x_1,...,x_i)\mathcal{W}^{(\kappa_{i+1}\cdots\kappa_n)}_{l_{i+1}\cdots l_n}(x_{i+1},...,x_n)$$

holds for $\lambda \to \infty$ *in the sense of convergence in* $\mathcal{S}'((\mathbb{R}^{1,3})^n)$.

From a theoretical point of view it is interesting to discuss to what extent these properties are connected to the axioms that imply them. In this respect one has the following important theorem [49]:

Theorem (Reconstruction). *Let* $\{\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n)\}$ *be a sequence of tempered distributions in* $\mathcal{S}'((\mathbb{R}^{1,3})^n)$ *which satisfy Properties 1–7. Then there exists a Hilbert space* $\mathcal{H}$*, a representation* $U(a,\alpha)$ *of* $\overline{\mathscr{P}^{\uparrow}_{+}}$ *in* $\mathcal{H}$*, a state* $|0\rangle \in \mathcal{H}$*, and fields* $\{\varphi^{(\kappa)}_l\}$ *such that:*

$$\langle 0|\varphi^{(\kappa_1)}_{l_1}(x_1)\cdots\varphi^{(\kappa_n)}_{l_n}(x_n)|0\rangle = \mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n)$$

and Axioms 1–6 are satisfied. Moreover, any other field theory which satisfies Axioms 1–6 and has Wightman functions that are equal to $\{\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n)\}$ *must be unitarily equivalent to this reconstructed theory.*

So the Reconstruction Theorem implies that a QFT satisfying Axioms 1–6 can be uniquely[15] reconstructed from the corresponding Wightman functions $\{\mathcal{W}^{(\kappa_1\cdots\kappa_n)}_{l_1\cdots l_n}(x_1,...,x_n)\}$. This is a powerful result and justifies why the vacuum expectation values of products of fields are the objects of central importance in QFT. Since any QFT satisfying Axioms 1–6 is describable in terms of its Wightman functions, which obey Properties 1–7, the implications of these axioms can therefore be explored by investigating the consequences of Properties 1–7. A selection of some of the more prominent consequences will be outlined during the remainder of this subsection.

Analyticity of the Wightman functions

Perhaps the most important structural relation implied by Properties 1–7 is that the Wightman functions[16] $W(\xi_1,...,\xi_{n-1})$ can be analytically continued beyond $(\mathbb{R}^{1,3})^{n-1}$. In particular, due to the Covariance (Property 2) and spectral condition (Property 3), one has the following theorem [49, 56]:

Theorem (Extended tube analyticity)**.** $W \in \mathcal{S}'((\mathbb{R}^{1,3})^{n-1})$ *is the boundary value of a function* $\mathbf{W}$ *in the sense that:*

$$W(\xi_1,...,\xi_{n-1}) = \lim_{\eta_1,...,\eta_{n-1}\to 0}\mathbf{W}(\xi_1 - i\eta_1,...,\xi_{n-1}-i\eta_{n-1}) \quad \textit{in } \mathcal{S}'$$

[15]This uniqueness is up to unitary equivalence, which is outlined in [49].
[16]The indices have been dropped here for simplicity.

and $\mathbf{W}$ *is holomorphic in* $T_{n-1} := (\mathbb{R}^{1,3} - iV^+)^{n-1}$*. Moreover,* $\mathbf{W}$ *has a unique analytic continuation* $\widetilde{\mathbf{W}}$ *into the extended tube* $T'_{n-1} := \bigcup_{\Lambda \in \mathscr{L}_+(\mathbb{C})} \Lambda T_{n-1}$*, where* $\mathscr{L}_+(\mathbb{C})$ *is the proper complex Lorentz group.*

It is important to point out here that the tube T_{n-1} does not contain any real points [56]. So although W is the boundary value of a (holomorphic) function $\mathbf{W}$ on T_{n-1}, this is not an analytic continuation of W since $\mathbf{W}$ is not defined on $(\mathbb{R}^{1,3})^{n-1}$ (in the sense of distributions). However, the extended tube T'_{n-1} *does* contain real points $J_{n-1} = T'_{n-1} \cap (\mathbb{R}^{1,3})^{n-1}$, called *Jost points* [49]. This means that $\widetilde{\mathbf{W}}$ defines an analytic continuation of W in a (complex) neighbourhood of the set $J_{n-1} \subset (\mathbb{R}^{1,3})^{n-1}$, and hence: $\widetilde{\mathbf{W}} \xrightarrow{\eta \to 0} W$ in this neighbourhood independently of whether $\eta \in V^+$ or $\eta \in V^-$ [49]. It is these structural relations which underpin the proofs of two of the most physically consequential theorems in axiomatic QFT – the *Spin-statistics theorem* [50] and *CPT theorem* [49]. Both of these theorems will be discussed in depth later on in this subsection. Since $\mathcal{W}(x_1, ..., x_n) = W(\xi_1, ..., \xi_{n-1})$, this means that $\widetilde{\mathbf{W}}$ also induces an analytic continuation $\widetilde{\boldsymbol{\mathcal{W}}}$ of $\mathcal{W}$ as follows:

$$\widetilde{\boldsymbol{\mathcal{W}}}(z_1, ..., z_n) = \widetilde{\mathbf{W}}(\zeta_1, ..., \zeta_{n-1}), \qquad \zeta = \xi - i\eta \in T'_{n-1}$$

and therefore $\widetilde{\boldsymbol{\mathcal{W}}}$ is holomorphic in $\mathscr{T}'_n := \{z \mid \zeta = (\zeta_1 = z_1 - z_2, ..., \zeta_{n-1}) \in T'_{n-1}\}$, which is often also referred to as the extended tube. The real (Jost) points of $\mathscr{T}'_n$ are then defined by $\mathscr{J}_n := \mathscr{T}'_n \cap (\mathbb{R}^{1,3})^n$.

As previously discussed, the covariance property and spectral condition imply that W has a holomorphic extension $\widetilde{\mathbf{W}}$ which is an analytic continuation of W around the Jost points J_{n-1}. A natural question to ask is whether any of the other properties satisfied by W imply that $\widetilde{\mathbf{W}}$ can be extended beyond T'_{n-1}? The answer is yes. Due to the locality of W (Property 4), one has the theorem [49, 56]:

Theorem (Symmetrised tube analyticity)**.** *The holomorphic extension* $\widetilde{\mathbf{W}}$ *of* W*, which is defined on* T'_{n-1}*, has an analytic continuation* $\widetilde{\mathbf{W}}_\pi$ *into the symmetrised tube* $T^S_{n-1} = \bigcup_{\pi \in S_{n-1}} \pi T'_{n-1}$*, where* S_{n-1} *is the group of permutations of the indices* $\{1, ..., n-1\}$*.*

From the definition of T^S_{n-1}, it is clear that $J_{n-1} \subset T^S_{n-1}$, and thus $\widetilde{\mathbf{W}}_\pi$ is also an analytic continuation of W. Moreover, due to the existence of $\widetilde{\boldsymbol{\mathcal{W}}}$ on $\mathscr{T}'_n$, $\widetilde{\mathbf{W}}_\pi$ induces an analytic continuation $\widetilde{\boldsymbol{\mathcal{W}}}_\pi(z_1, ..., z_n)$ of $\mathcal{W}(x_1, ..., x_n)$, which is holomorphic in $\mathscr{T}_n^S = \bigcup_{\pi \in S_n} \pi \mathscr{T}_n'$ (symmetrised tube). In this context, given $(z_1, ..., z_n) \in \mathscr{T}_n'$, one defines $\pi(z_1, ..., z_n) := (z_{\pi(1)}, ..., z_{\pi(n)})$. An important concept in QFT is the notion of *Euclidean points* [47]. A *real* Euclidean point is defined by:

$$y = (y_1, ..., y_n), \qquad y_i = (\tau_i, \mathbf{x}_i) \in \mathbb{E} = \mathbb{R}^4$$

and thus $y \in \mathbb{E}^n$. A *complex* Euclidean point $z \in (\mathbb{C}^{1,3})^n$ has the form:

$$z = (z_1, ..., z_n), \qquad z_i = (i\tau_i, \mathbf{x}_i) \in \mathbb{C}^{1,3}$$

It is clear that the correspondence $y \leftrightarrow z$ between real and complex Euclidean points is one-to-one. In the case where $y_i \neq y_j$ for all $i \neq j$, and hence $z_i \neq z_j$ for all $i \neq j$, $z = (z_1, ..., z_n)$ is called a *non-coincident* (complex) Euclidean point. It turns out that one has the following theorem:

Theorem (Euclidean analyticity)**.** *The symmetrised tube $\mathscr{T}_n^S$ contains all of the non-coincident complex Euclidean points z, and hence the analytic continuation $\widetilde{\boldsymbol{\mathcal{W}}}_\pi(z_1, ..., z_n)$ of the Wightman function $\mathcal{W}(x_1, ..., x_n)$ is well-defined at these points.*

This theorem enables one to define the Euclidean analogue $\mathcal{S}(y_1, ..., y_n)$ of the Minkowski Wightman functions, called the *Schwinger functions*. The Schwinger functions are defined by:

$$\mathcal{S}(y_1, ..., y_n) := \widetilde{\boldsymbol{\mathcal{W}}}_\pi(z_1, ..., z_n), \;\; \textit{where } z \textit{ is a non-coincident complex Euclidean point}$$

The fact that $\mathcal{S}(y_1, ..., y_n)$ are well-defined provides mathematical justification to the heuristic procedure of replacing τ with imaginary time $i\tau$, which is the inverse of the so-called *Wick transformation* $\tau \to -i\tau$. So given an axiomatic QFT in Minkowski spacetime, these results demonstrate that the Euclidean theory is guaranteed to exist. The Schwinger functions $\{\mathcal{S}(y_1, ..., y_n)\}$ form the structural foundation of any Euclidean QFT, and can be shown to satisfy the so-called *Osterwalder-Schrader* axioms, which are the Euclidean counterparts of Properties 1–7 [47]. Moreover, the converse statement holds; given Schwinger functions[17] $\mathcal{S}(y_1, ..., y_n) \in \mathcal{S}'_{\neq}(\mathbb{E}^n)$ that satisfy the

[17] Since $\mathcal{S}(y_1, ..., y_n)$ is only defined at non-coincident Euclidean points, it is a distribution on the space of test functions $\mathcal{S}_{\neq}(\mathbb{E}^n) := \{f \in \mathcal{S}(\mathbb{E}^n) \mid D^k f(y_1, ..., y_n) = 0, \forall k \text{ when } y_i = y_j \text{ for any } i \neq j\}$.

Osterwalder-Schrader axioms, $\mathcal{S}(y_1, ..., y_n)$ define Wightman functions which possess Properties 1–7, and hence (by the Reconstruction Theorem) imply the existence of a relativistic QFT that obeys Axioms 1–6 [63, 64]. This is an extremely powerful result because it implies that relativistic and Euclidean QFTs which satisfy certain axioms, are completely equivalent to one another. In many cases, the corresponding objects in the Euclidean theory have simpler mathematical properties, and thus this equivalence allows one to first solve problems in the Euclidean theory, and then perform a Wick transformation ($\tau \to -i\tau$) in order to recover the corresponding relativistic solution. An important example of this is the path integral formulation of QFT. It turns out that the path integral itself is mathematically ill-defined in the Minkowski regime [47]. However, in Euclidean spacetime it *is* possible to define this object in a rigorous manner. This formalism can then be used both as a non-perturbative calculation tool, such as in lattice QFT [53], and also as a method for actually explicitly proving the existence of certain QFT models[18] [55].

The Reeh-Schlieder theorem and separating property of the vacuum

The analyticity properties discussed previously have many implications. Two consequences which are technical, but particularly consequential, are the *Reeh-Schlieder Theorem* and the separating property of the vacuum. The Reeh-Schlieder Theorem is defined as follows [65]:

Theorem (Reeh-Schlieder)**.** *Let $\mathcal{O} \subset \mathbb{R}^{1,3}$ be any open set, and $\mathcal{F}(\mathcal{O})$ denote the polynomial algebra of fields smeared with test functions with support in $\mathcal{O}$. Then $|0\rangle$ is a cyclic vector for $\mathcal{F}(\mathcal{O})$, and hence $\mathcal{F}(\mathcal{O})|0\rangle$ is dense in $\mathcal{H}$ (i.e. $\mathcal{H} = \overline{\mathcal{F}(\mathcal{O})|0\rangle}$).*

This theorem has some surprising consequences. For example, no matter how small the region $\mathcal{O} \subset \mathbb{R}^{1,3}$ is, any state in[19] $\mathcal{H} := \overline{\mathcal{F}(\mathbb{R}^{1,3})|0\rangle}$ can be approximated by states localised in $\mathcal{O}$. Moreover, if one considers some region $\mathcal{O}'$ to be space-like separated to $\mathcal{O}$, then the cluster property (Property 7) implies that the correlations between states in $\mathcal{F}(\mathcal{O}')|0\rangle$ and $\mathcal{F}(\mathcal{O})|0\rangle$ become increasingly smaller the further away that $\mathcal{O}$

[18] This approach is often called *constructive field theory* [55].

[19] This definition of $\mathcal{H}$ follows from Axiom 4.

and $\mathcal{O}'$ are separated. Therefore, with respect to measurements in $\mathcal{O}'$, the states in $\mathcal{O}$ effectively look like the vacuum, and so are in some sense localised. However, due to the Reeh-Schlieder theorem it follows that for any state $|\Psi\rangle$ in $\mathcal{O}$, there exists some operator $Q \in \mathcal{F}(\mathcal{O}')$ which when applied to $|0\rangle$ produces a state arbitrarily close to $|\Psi\rangle$. So although the cluster property gives some qualitative notion of localised states, the Reeh-Schlieder theorem ensures that there always exists non-vanishing long distance correlations in the vacuum [50]. The concept of localisation is therefore a subtle issue in QFT.

The separating property of the vacuum is a corollary of the Reeh-Schlieder theorem, and is summarised as follows [65]:

Theorem. *Let $\mathcal{O} \subset \mathbb{R}^{1,3}$ be any open set for which there exists an open set $\mathcal{O}'$ which is non-empty and space-like with respect to $\mathcal{O}$. If $A \in \mathcal{F}(\mathcal{O})$ and $A|0\rangle = 0$, then $A = 0$.*

An immediate consequence of this theorem is that the algebra $\mathcal{F}(\mathcal{O})$ cannot contain non-trivial number operators or charge operators such as P^μ, since they annihilate the vacuum. The physical interpretation, much like with the Reeh-Schlieder theorem, is that it is not possible to measure states in QFT in a localised manner. In other words, it is difficult to completely isolate a system described by quantised fields from outside effects [49].

Field quantisation

The procedure of quantising a field theory by requiring that the fields satisfy specific equal-time (anti-)commutation relations is in general inconsistent [47, 52]. This inconsistency lies in the fact that quantised fields are operator-valued distributions, not functions, and hence cannot be assumed to be point-wise defined. In particular, for interacting QFTs (in $\mathbb{R}^{1,3}$) the fields are not defined at sharp times, and thus equal-time (anti-)commutation relations cannot be imposed [47]. This failure of the canonical quantisation procedure poses an important question: *can field theories be quantised in a rigorous manner?* Although the construction of realistic QFTs is an ongoing problem, the Wightman axioms (and hence Properties 1–7) have been shown in many instances to be a consistent framework in which to quantise field theories [55]. The simplest class of QFTs involve fields with no interactions. In this case one has the following theorem [47, 66]:

Theorem (Jost and Schroer). *If a free field theory obeys the Wightman axioms, this implies that the fields in the theory satisfy canonical equal-time (anti-)commutation relations.*

This theorem therefore demonstrates that the Wightman axioms actually reproduce the canonical quantisation structure of free theories, and hence qualify as a substitute for this procedure. Although the Wightman axioms may require modifications in order to describe certain classes of QFTs (see Sec. 1.2.4), the fact that both free and interacting theories[20] can be shown to satisfy these axioms is strong evidence to suggest that at least the essence of this non-perturbative quantisation approach is correct.

The Spin-statistics theorem

The Spin-statistics theorem is an important result that establishes the connection between the commutativity and Lorentz transformation properties of a field. The most general form of the theorem is defined as follows [47, 49]:

Theorem (Spin-statistics). *Let $\varphi^{(\kappa)}$ be a field which transforms as a finite irreducible $\left(\frac{j}{2}, \frac{k}{2}\right)$ representation of $\overline{\mathscr{L}_+^\uparrow} \cong \mathrm{SL}(2,\mathbb{C})$, and hence has integer/half-odd integer spin when $j+k$ is even/odd. Then the following connection of spin and statistics:*

$$\begin{aligned} \left[\varphi^{(\kappa)}(x), (\varphi^{(\kappa)})^*(y)\right]_+ &= 0, \quad \textit{if } \varphi^{(\kappa)} \textit{ has integer spin} \\ \left[\varphi^{(\kappa)}(x), (\varphi^{(\kappa)})^*(y)\right]_- &= 0, \quad \textit{if } \varphi^{(\kappa)} \textit{ has half-odd integer spin} \end{aligned}$$

for $x-y$ space-like, implies that $\varphi^{(\kappa)}(f)|0\rangle = \varphi^{(\kappa)}(f)^*|0\rangle = 0 \ \forall f \in \mathcal{S}(\mathbb{R}^{1,3})$. If all fields either commute or anti-commute, then it further follows that: $\varphi^{(\kappa)} = (\varphi^{(\kappa)})^* = 0$.

As mentioned in Sec. 1.2.3, the analytic properties of the Wightman functions play an important role in the proof of this theorem, as we will now discuss. Consider an

[20] For example, the interacting ϕ^4-theory has been proven to exist and satisfy the Wightman axioms [55].

arbitrary (complex) field $\varphi^{(\kappa)}$ which transforms as a finite irreducible $\left(\frac{j}{2}, \frac{k}{2}\right)$ representation. By assumption, $\varphi^{(\kappa)}$ satisfies the property $\left[\varphi^{(\kappa)}(x), (\varphi^{(\kappa)})^{*}(y)\right]_{\pm} = 0$ for $x-y$ space-like, and $\pm = (-1)^{j+k}$. It follows that:

$$\langle 0|\varphi^{(\kappa)}(x)(\varphi^{(\kappa)})^{*}(y)|0\rangle + (-1)^{j+k}\langle 0|(\varphi^{(\kappa)})^{*}(y)\varphi^{(\kappa)}(x)|0\rangle = W_1(\xi) + (-1)^{j+k}W_2(-\xi) = 0$$

where $\xi = x-y$. Since ξ is a space-like vector, this means that ξ is a *Jost point*, and thus from the analysis in Sec. 1.2.3 both W_1 and W_2 possess unique analytic continuations, $\widetilde{\mathbf{W}}_1$ and $\widetilde{\mathbf{W}}_2$, which are defined in the extended tube T_1'. The previous equality therefore implies:

$$\widetilde{\mathbf{W}}_1(\zeta) + (-1)^{j+k}\widetilde{\mathbf{W}}_2(-\zeta) = 0, \qquad \zeta \in T_1'$$

Furthermore, by construction, these analytic continuations are invariant under proper complex Lorentz transformations $\mathscr{L}_{+}(\mathbb{C})$. In particular, in this case this means that $\widetilde{\mathbf{W}}_2(-\zeta) = (-1)^{j+k}\widetilde{\mathbf{W}}_2(\zeta)$. Combining these results one has:

$$\begin{aligned}\lim_{\eta\to 0}\left[\widetilde{\mathbf{W}}_1(\zeta) + (-1)^{j+k}\widetilde{\mathbf{W}}_2(-\zeta)\right] &= \lim_{\eta\to 0}\left[\widetilde{\mathbf{W}}_1(\zeta) + \widetilde{\mathbf{W}}_2(\zeta)\right] \\ &= \langle 0|\varphi^{(\kappa)}(x)(\varphi^{(\kappa)})^{*}(y)|0\rangle + \langle 0|(\varphi^{(\kappa)})^{*}(-y)\varphi^{(\kappa)}(-x)|0\rangle = 0\end{aligned}$$

for all $x, y \in \mathbb{R}^{1,3}$. Finally, since $(\varphi^{(\kappa)})^{*}(f) = [\varphi^{(\kappa)}(\bar{f})]^{*}$, and setting $\hat{f}(x) = f(-x)$ where $f \in \mathcal{S}(\mathbb{R}^{1,3})$, one can write:

$$\begin{aligned}\int d^4x\, d^4y f(x)\overline{f(y)}\ \Big[\langle 0|\varphi^{(\kappa)}(x)(\varphi^{(\kappa)})^{*}(y)|0\rangle &+ \langle 0|(\varphi^{(\kappa)})^{*}(-y)\varphi^{(\kappa)}(-x)|0\rangle\Big] \\ &= \langle 0|\varphi^{(\kappa)}(f)\varphi^{(\kappa)}(f)^{*}|0\rangle + \langle 0|\varphi^{(\kappa)}(\hat{f})^{*}\varphi^{(\kappa)}(\hat{f})|0\rangle \\ &= ||\varphi^{(\kappa)}(f)^{*}|0\rangle||^2 + ||\varphi^{(\kappa)}(\hat{f})|0\rangle||^2 = 0\end{aligned}$$

and thus: $\varphi^{(\kappa)}(f)|0\rangle = \varphi^{(\kappa)}(f)^{*}|0\rangle = 0$. If $\varphi^{(\kappa)}$ is contained in a theory in which all of the fields either commute or anti-commute, then it follows from the separating property of the vacuum (in Sec. 1.2.3) that: $\varphi^{(\kappa)} = (\varphi^{(\kappa)})^{*} = 0$.

To appreciate the physical relevance of the Spin-statistics theorem, it is important to understand the constraints it imposes on quantum mechanical systems. In (non-relativistic) quantum mechanics, a state of N particles consists of identical particles if and only if all observables remain invariant under the interchange of any particle labels describing the state. This implies that pure N-particle states are one-dimensional representations of the group of permutations S_N [47]. It turns out that there are two such possibilities: the trivial (symmetric) representation, and the non-trivial (anti-symmetric) representation. States in the trivial representation are referred to as having *Bose-Einstein statistics*, and in the non-trivial representation as having *Fermi-Dirac statistics.* In QFT, states with symmetric or anti-symmetric statistics are described by fields which respectively commute or anti-commute at space-like separated points. The Spin-statistics theorem essentially states that a non-trivial integer/half-odd integer spin field cannot have an anti-commutator/commutator which vanishes for space-like separations respectively. Therefore, if one assumes that Bose-Einstein and Fermi-Dirac are the only allowed statistics that a system can possess[21], the Spin-statistics theorem implies that: *integer spin systems obey Bose-Einstein statistics and half-odd integer spin systems obey Fermi-Dirac statistics.* This connection between spin and statistics is a truly profound result because it explains the origin of one of the most important principles in physics – the *Pauli-exclusion principle* [67]. It is quite remarkable that by using an axiomatic QFT approach, which consists of only a few physically motivated axioms, one can actually derive the principle that explains the existence of different chemical elements in the universe and the stability of matter [68]. The Spin-statistics theorem has been experimentally tested using a wide variety of different approaches [69]. Some examples of these tests include searching for: Bose-Einstein symmetry violating two photon decays [70], violations of permutation symmetry in nuclei [71], and Pauli-exclusion principle violating atomic transitions [72]. Despite the precision and range of these and other experiments, no significant violation of the Spin-statistics theorem has ever been observed [69].

The CPT theorem

The CPT theorem[22] concerns the combined symmetry of CPT, which is the product of the following symmetries:

- charge conjugation C (reversal of charge)

[21]Technically, other possible statistics are possible (para-statistics) [50], but we will not discuss these here.

[22]In different conventions this is also referred to as the PCT theorem [47, 49].

- parity P (inversion of spatial coordinate: $\mathbf{x} \to -\mathbf{x}$)
- time reversal T (reversal of time: $t \to -t$)

The precise definition of how these individual symmetries are implemented as operators on different fields is convention dependent[23]. Nevertheless, one has the following general theorem [49, 50]:

Theorem (CPT). *CPT is a symmetry of any QFT that satisfies the Wightman axioms, and is implemented by a unique anti-unitary operator* Θ *which has the following properties:*

$$\Theta\,\varphi^{(\kappa)}(x)\,\Theta^{-1} = (-1)^j i^{F^{(\kappa)}} (\varphi^{(\kappa)})^*(-x)$$
$$\Theta|0\rangle = |0\rangle$$
$$F^{(\kappa)} = \begin{cases} 0, & j+k \textit{ is even} \\ 1, & j+k \textit{ is odd} \end{cases}$$

where the field $\varphi^{(\kappa)}$ *transforms as a finite irreducible* $\left(\frac{j}{2}, \frac{k}{2}\right)$ *representation of* $\mathrm{SL}(2, \mathbb{C})$*.*

Similarly to the Spin-statistics theorem, the analytic properties of the Wightman functions are also important in the proof of the CPT theorem. The theorem can be proven in a straight-forward manner by using the fact that the existence of an operator Θ, which satisfies the properties outlined above, is equivalent to the validity of the condition [49]:

$$W^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\xi_1, ..., \xi_{n-1}) = (-1)^J i^F W^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(\xi_{n-1}, ..., \xi_1)$$

where $J = \sum_{a=1}^n j_a$ ($\varphi^{(\kappa_a)}$ has $j = j_a$) and $F = \sum_{a=1}^n F^{(\kappa_a)}$. Consider the situation where $\xi_i = x_i - x_{i+1}$ are all *space-like* vectors. Due to Property 4, it follows that one can write[24]:

$$\begin{aligned} W^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\xi_1, ..., \xi_{n-1}) = \mathcal{W}^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(x_1, ..., x_n) &= i^F \mathcal{W}^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(x_n, ..., x_1) \\ &= i^F W^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(-\xi_{n-1}, ..., -\xi_1) \end{aligned}$$

[23] A discussion of this issue can be found in [49].

[24] See [47, 49] for more details.

Moreover, since ξ_i are all space-like it must be that $\xi = (\xi_1, ..., \xi_{n-1})$ is a Jost point (i.e. $\xi \in J_{n-1}$). $W^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\xi_1, ..., \xi_{n-1})$ therefore has a unique analytic continuation $\widetilde{\mathbf{W}}^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\zeta_1, ..., \zeta_{n-1})$ to the extended tube T'_{n-1}, and hence, due to the equality above, the following condition must hold:

$$\widetilde{\mathbf{W}}^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\zeta_1, ..., \zeta_{n-1}) = i^F \widetilde{\mathbf{W}}^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(-\zeta_{n-1}, ..., -\zeta_1), \quad \zeta \in T'_{n-1}$$

By construction, $\widetilde{\mathbf{W}}$ is invariant under proper complex Lorentz transformations $\mathscr{L}_+(\mathbb{C})$, and this means in particular that:

$$\widetilde{\mathbf{W}}^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(-\zeta_{n-1}, ..., -\zeta_1) = (-1)^J \widetilde{\mathbf{W}}^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(\zeta_{n-1}, ..., \zeta_1)$$

Finally, by combining these results one has:

$$\begin{aligned} W^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\xi_1, ..., \xi_{n-1}) &= \lim_{\eta_1, ..., \eta_{n-1} \to 0} \widetilde{\mathbf{W}}^{(\kappa_1 \cdots \kappa_n)}_{l_1 \cdots l_n}(\zeta_1, ..., \zeta_{n-1}) \\ &= (-1)^J i^F \lim_{\eta_1, ..., \eta_{n-1} \to 0} \widetilde{\mathbf{W}}^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(\zeta_{n-1}, ..., \zeta_1) \\ &= (-1)^J i^F W^{(\kappa_n \cdots \kappa_1)}_{l_n \cdots l_1}(\xi_{n-1}, ..., \xi_1) \end{aligned}$$

for all $\xi \in (\mathbb{R}^{1,3})^{n-1}$, which proves the existence of the CPT operator Θ.

Perhaps the most striking consequence of this theorem is that the operator Θ transforms a single particle state $|\Psi\rangle$ into a state $|\overline{\Psi}\rangle$ with the same mass and spin, but opposite quantum numbers. So for every particle state $|\Psi\rangle$, there also exists a corresponding *anti-particle* state $|\overline{\Psi}\rangle$. In other words, the CPT theorem predicts the existence of anti-particles[25]. A remarkable feature of this result is that CPT is guaranteed to *always* be a symmetry of the theory, independently of whether C, P or T are individually symmetries themselves. So CPT symmetry and the existence of anti-particles is a ubiquitous feature of any QFT which satisfies the Wightman axioms. Many different experimental searches for CPT violation have been performed, including measurements of the mass difference between particles and anti-particles [12, 69] and the search for CPT violating decays [73], and all of these findings support the hypothesis that CPT is a conserved symmetry. Another important consequence of the CPT theorem is that if either one of the C, P or T symmetries are violated, it must be the case that at least one of the other symmetries is also violated, in order to ensure that the overall

[25] It may well be the case that $|\Psi\rangle = |\overline{\Psi}\rangle$, in which case it is referred to as a Majorana state [50].

CPT symmetry is preserved [69]. A prominent example of this is the violation of CP symmetry[26], which subsequently implies the non-conservation of time reversal T symmetry.

1.2.4 Local quantisation

From the discussions in the Sec. 1.2.3 it is clear that the Wightman axioms provide a powerful framework from which one can rigorously define QFTs. However, it transpires that these axioms are not completely sufficient for describing an important class of QFTs – *gauge theories*. For a classical field theory, a gauge symmetry is a localisation of some global symmetry. More precisely, given some n-dimensional Lie group G, a field φ has the following infinitesimal transformation[27] [47]:

$$\delta\varphi_i(x) = i\varepsilon_a T^a_{ij}\varphi_j(x)$$

where ε_a $(a = 1, ..., n)$ are group parameters, and T^a_{ij} $(i, j = 1, ..., d)$ is a d-dimensional representation of the basis $\{T^a\}$ of elements (generators) of the Lie algebra Lie(G) of G. An *infinitesimal gauge transformation* is a generalisation of this class of symmetries in which ε_a are no longer constants, but are instead regular functions $\varepsilon_a(x)$. The space of all such transformations forms an infinite-dimensional Lie algebra Lie$(\mathcal{G})$ of a group $\mathcal{G}$, and $\mathcal{G}$ is called the *local gauge group* associated with G. An important property of gauge theories is the necessity to introduce fields $\{A^a_\mu\}$ (gauge fields). These fields are defined to transform under infinitesimal gauge transformations in the following manner:

$$\delta^\varepsilon A^b_\mu(x) = i\varepsilon_a T^a_{bc} A^c_\mu(x) + \partial_\mu \varepsilon^b(x)$$

where T^a_{bc} is the adjoint representation of $\{T^a\}$. If one naively applied *Noether's (First) Theorem*, this would suggest that invariance under the infinite-dimensional gauge group $\mathcal{G}$ implies an infinite set of conserved currents. Instead, invariance under infinitesimal

[26] The phenomenon of CP violation was first observed by [74].

[27] For simplicity it is assumed here that G is compact, the coupling parameter is absorbed in the definition of T^a, and that the symmetry is *internal*, and hence does not act on the spacetime argument of $\varphi(x)$.

gauge transformations implies the *local Gauss law* [47]:

$$J^a_\mu = \partial^\nu G^a_{\mu\nu}, \quad G^a_{\mu\nu} = -G^a_{\nu\mu}$$

where J^a_μ is the current associated with invariance under the global (charge) group G. The local Gauss law is a strengthened form of the conservation law for J^a_μ because due to the anti-symmetry of $G^a_{\mu\nu}$, $\partial^\mu J^a_\mu = 0$ holds independently of the equations of motion. When a field theory is quantised it is not guaranteed that all of the features of the corresponding classical theory will continue to hold. This is a central theme of Chaps. 2 and 3. In particular, for quantised gauge theories the transformation $\delta^\varepsilon A^b_\mu$ itself needs a suitable operator interpretation, i.e. $\varepsilon^b(x)$ can no longer be an arbitrary regular function, otherwise this would violate the relativistic covariance (Axiom 5) of the fields A^a_μ. Moreover, even with this definition, it transpires that not all gauges can be connected by transformations of this form [75]. Because the structure of gauge invariance is really quite different for quantised theories, this poses an important question: *what is the characteristic feature of a quantised gauge theory?* Although this still remains an open problem, there is evidence to suggest that it is the local Gauss law (as an operator equation) which captures the essential features of a gauge theory, and that local gauge invariance is simply a procedure for constructing Lagrangians which lead to the validity of local Gauss laws [47].

The existence of local Gauss laws is fundamental to the prediction of many important phenomena in quantum gauge field theories, including the evasion of *Goldstone's Theorem* (i.e. the Higgs mechanism) [76], confinement [77, 78], and the properties of charged states [75]. All of these feature arise because the structure of the charge[28] Q^a corresponding to the current J^a_μ implies the following theorem [79]:

Theorem. *A field that transforms non-trivially with respect to Q^a is non-local.*

Non-locality here means that the field fails to satisfy local (anti-)commutativity (Axiom 6). This theorem has the important consequence that charged fields are non-local, which implies that charged *states* cannot be contained in (the closure of) $\mathcal{F}|0\rangle$, where $\mathcal{F}$ is a local field algebra, and so are in this sense non-local [79]. As outlined in Chap. 2, this feature of local Gauss laws implies that there are effectively two approaches for

[28]The definition of the charge Q^a and its transformation on fields is described in Chaps. 2 and 3.

defining a quantised gauge theory. In the first approach one assumes that the local Gauss law holds exactly as an operator equation, which implies that field algebra is non-local, but that the Hilbert space structure defined by Axiom 1 is preserved. An example of this approach is the Coulomb gauge quantisation of QED, where the electron field is subsequently non-local [47]. The other approach involves modifying the local Gauss law in order to preserve the locality of the fields. However, this procedure implies that the space of states $\mathcal{V}$ can no longer have a positive-definite inner product[29], and so requires a modification of the Wightman axioms [47, 51, 56, 77, 78]. Gauge theories which are *locally quantised* achieve a modification of the local Gauss law by adding additional degrees of freedom into the theory. An important example is the *BRST quantisation* of QCD, where gauge-fixing and (Faddeev-Popov) ghost fields are introduced [51], and the additional states associated with these fields are included in $\mathcal{V}_{\mathrm{QCD}}$. Since $\mathcal{V}_{\mathrm{QCD}}$ necessarily contains unphysical (negative norm) states, one requires a (subsidiary) condition in order to characterise the physical states $\mathcal{V}_{\mathrm{phys}} \subset \mathcal{V}_{\mathrm{QCD}}$. This condition corresponds to the requirement that the local Gauss law is preserved for physical states $|\Psi\rangle \in \mathcal{V}_{\mathrm{phys}}$, and hence:

$$\langle \Psi | J^{a}_{\mu} - \partial^{\nu} G^{a}_{\mu\nu} | \Psi \rangle = 0, \quad \forall \, |\Psi\rangle \in \mathcal{V}_{\mathrm{phys}}$$

This is often referred to as the *weak Gauss law* [47]. Due to the modification of the local Gauss law the theory is no longer gauge-invariant, but remains invariant under a residual *BRST symmetry*, which has an associated charge Q_B [80]. It turns out that under the assumption that Q_B is unbroken (and hence $Q_B|0\rangle = 0$), the condition $Q_B \mathcal{V}_{\mathrm{phys}} = 0$ is equivalent to the weak Gauss law. The corresponding physical Hilbert space is then defined by $\mathcal{H}_{\mathrm{QCD}} := \overline{\mathcal{V}_{\mathrm{phys}}/\mathcal{V}_0}$, where $\mathcal{V}_0 \subset \mathcal{V}_{\mathrm{phys}}$ are the zero norm states, and the closure guarantees that certain limit states[30] are also contained in $\mathcal{H}_{\mathrm{QCD}}$.

Although local quantisations require the introduction of additional degrees of freedom, the locality of the field algebra is preserved, which has the advantage that many of the structural and physical consequences derived from the Wightman axioms, some of which are discussed in Sec. 1.2.3, continue to hold [47, 78]. It is for this reason that

[29] Since $\mathcal{V}$ no longer has a positive-definite inner product, it is instead assumed to have the structure of a pseudo-Hilbert space [56].

[30] See [51, 56] for a discussion of the structure of the pseudo-Hilbert space $\mathcal{V}_{\mathrm{QCD}}$ used to define these limit states.

local quantisations play a prominent role in the discussions in this thesis, particularly in Chaps. 2, 3 and 5.

Overview of Chapters 2 and 3

As the title suggests, this thesis is comprised of a series of investigations into different aspects of non-perturbative QFT. The overarching theme of these investigations concerns the application of axiomatic QFT in order to gain new insights into unresolved problems in particle physics. In particular, Chaps. 2 and 3 address the issue of how to define spatial boundary operators $\int d^3x\, \partial_i B^i$ in a consistent manner, and why this plays a central role in the context of many important physical problems. Chaps. 2 and 3 correspond to the publications [1] and [3] respectively, and are therefore self-contained research articles. Since these articles have inter-related content, they necessarily contain overlap, in particular with regards to some of the definitions and arguments. Moreover, these article were written with a view to brevity and clarity, and so the background context is deliberately kept concise. Therefore, in order to further motivate the relevance of these works, in this section I will describe the context of these works with regards to the literature and the key issues involved.

For several decades a disagreement has been raging in the particle and nuclear physics community as to how nucleons get their spin [81–89]. This disagreement centres around a key question: *does the spin of a nucleon arise due to the spin of its quark and gluon constituents?* If yes, then in principle it should be possible to individually measure these spin contributions, and test whether the spin of a polarised hadron, such as a proton, is equal to the sum of the spin of its constituents. As detailed in Chap. 2, it turns out that this issue crucially depends on whether the expression for the angular momentum operator in QCD, J^i_{QCD}, can be meaningfully decomposed in such a way that each of the pieces in the decomposition corresponds to a quark or gluon angular momentum observable. These operators are then inserted between polarised hadronic states in order to form a sum rule. A case of particular experimental interest is when these states are polarised proton states, since one obtains the following sum rule [81, 83]: $\frac{1}{2} = \frac{1}{2}\Sigma + L_q + S_g + L_g$, where Σ, S_g and L_q, L_g are interpreted as measuring the contribution to the intrinsic spin and orbital angular momentum of the proton from the quarks and gluons respectively[31].

In the literature, it is generally believed that each of the terms in this decomposition is measurable, although only the terms Σ and S_g have so far been measured [89]. In 1988, the European Muon Collaboration (EMC) performed polarised deep-inelastic muon-proton scattering in order to measure Σ. They found that Σ was small [90], which contradicted the belief at the time that quarks accounted for the majority of the spin of the proton – the so called *proton spin crisis*. In the proceeding years, the focus has shifted on trying to measure the other pieces of the sum rule, with the motivation being that the crisis can be resolved if the rest of the proton's spin comes from the orbital terms and S_g. Currently, there are experimental collaborations all over the world, including COMPASS, STAR and PHENIX, which are attempting to perform these measurements. In particular, these collaborations have focussed on the measurement of the supposed gluon contribution to the intrinsic spin of the proton, S_g. The possibility to measure S_g comes from the fact that it can be written in the form: $S_g = \int_0^1 dx\, [G_+(x) - G_-(x)] = \int_0^1 dx\, \Delta G(x)$, where $G_\pm$ are the polarised gluon parton distribution functions[32]. By measuring observables such as the double-helicity asymmetry $A_{LL} = \Delta\sigma/\sigma$, where σ ($\Delta\sigma$) is the unpolarised (polarised) cross-section for a given proton-proton collision process, this data can be used to constrain the form of $\Delta G(x)$, and hence determine S_g [91]. Recent results from both STAR [92] and PHENIX [91] conclude that S_g is comparable to Σ, and according to the sum rule this therefore suggests that the remainder of the spin must be contained in the terms L_g and L_q.

Although the quantities Σ and S_g are measured in experiments, the solution to the proton spin crisis assumes that the decomposition of J^i_{QCD}, and the corresponding sum rule, are theoretically valid. It turns out that there are in fact many possible decompositions of J^i_{QCD}[33], and a common feature of all of these decompositions is that

[31] See Chap. 2 for more details.
[32] See [45] for a precise definition of these quantities.
[33] See [89] for a review of these decompositions.

they require one to assume that spatial boundary operators of the form $\int d^3x\, \partial_i B^i$ always vanish. This is justified by invoking Stokes' Theorem and imposing certain boundary conditions on the fields. However, by making this assumption one fails to take into account an important feature of QFT – quantum fields are distributions[34] and not functions, like in classical field theories. In Chap. 2 it is explicitly demonstrated that if one does take into account the distributional behaviour of quantum fields, the issue of whether $\int d^3x\, \partial_i B^i$ vanishes or not is more subtle than in the classical case. Moreover, it is argued that by treating spatial boundary operators in a rigorous manner, this enables one to determine which (if any) of the J^i_{QCD} decompositions are physically valid, and therefore whether it is in fact meaningful at all to measure the spin structure of hadrons in experiments such as COMPASS, STAR and PHENIX.

In Chap. 3 spatial boundary operators are again investigated, but this time in the context of non-manifest symmetries and their quantisation. Classical non-manifest symmetries are symmetries for which the variation of the Lagrangian density $\mathcal{L}$ is non-vanishing. In particular, $\mathcal{L} = \partial_\mu \mathcal{B}^\mu$, which implies an ambiguity in the definition of the conserved currents j^μ, and hence also the charges $Q = \int d^3x\, j^0$ associated with this class of symmetries. This ambiguity essentially boils down to the freedom of being able to redefine Q by adding a suitable spatial boundary term. Therefore, when a field theory that possesses a non-manifest symmetry is quantised, the issue of whether there is in fact a freedom in the definition of Q depends on if Q is non-trivially modified by adding spatial boundary *operators* of the form $\int d^3x\, \partial_i B^i$. This question is of profound importance since it has the potential to destroy the uniqueness of the charge Q, which in turn can affect the consistency of many features of quantum non-manifest symmetries, including: spontaneous symmetry breaking, the role of Q as the generator of the corresponding symmetry transformation, and the action of Q on states. Moreover, since several of the most important symmetries in QFT are non-manifest (e.g. translational invariance, Lorentz invariance, supersymmetry), this further motivates why it is crucial to understand the effects of Q being possibly non-unique.

An important example which illustrates these issues is translational invariance. Ever since the discovery by Belinfante [93] that the energy-momentum operator P^μ_B can instead be defined from a *symmetric* energy-momentum tensor $T^{\mu\nu}_B := T^{\mu\nu}_c + \partial_\rho G^{[\mu\rho]\nu}$,

[34] The physical motivation for this feature is discussed in Sec. 1.2, as well Chaps. 2 and 3.

where $T_c^{\mu\nu}$ is the canonical current derived from Noether's Theorem, it has remained unclear which of P_B^μ or P_c^μ (if either) is the correct expression for P^μ. Discussions in the literature which have tried to address this issue mostly arrive at the conclusion that either of these operators is meaningful, since one can apply Stokes' Theorem to the spatial boundary term $\int d^3x \, \partial_\rho G^{[0\rho]\nu}$, and by applying suitable boundary conditions this term vanishes [42, 44, 94, 95]. This is precisely the same argument encountered in Chap. 2 with regards to the viability of the decompositions of J^i_{QCD}. However, as mentioned previously, this argument is not valid because it ignores the distributional behaviour of the fields. Therefore, one cannot necessarily assume that P_B^μ and P_c^μ are equal, nor that they are both valid energy-momentum operators. In principle this means that P_c^μ could generate (infinitesimal) spacetime translations of the fields φ, i.e. $i[P_c^\mu, \varphi] = \delta\varphi$, whereas P_B^μ might not. Even more concerning, it could be that P_c^μ is preserved, whereas P_B^μ is spontaneously broken. In other words, one might not be able to definitely conclude if the symmetry is spontaneously broken or not, and thus determine whether the QFT in question is stable! More directly, if P_B^μ and P_c^μ where found to not be equal operators, then this would necessarily imply that their action on states is not the same, and therefore they certainly could not both be considered valid energy-momentum operators. All of these important issues will be addressed in general in Chap. 3, but the particular case of the energy-momentum operator is also discussed in Sec. 2.7.

Chapter 2

Boundary terms in quantum field theory and the spin structure of QCD

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2.1 Abstract

Determining how boundary terms behave in a quantum field theory (QFT) is crucial for understanding the dynamics of the theory. Nevertheless, boundary terms are often neglected using classical-type arguments which are no longer justified in the full quantum theory. In this paper we address this problem by establishing a necessary and sufficient condition for arbitrary spatial boundary terms to vanish in a general QFT. As an application of this condition we examine the issue of whether the angular momentum operator in Quantum Chromodynamics (QCD) has a physically meaningful quark-gluon decomposition. Using this condition it appears as though this is not the case, and that it is in fact the non-perturbative QCD structure which prevents the possibility of such a decomposition.

2.2 Introduction

When classical and quantum field theories are discussed it is often assumed that spatial boundary terms do not contribute [42, 44, 95–97]. The standard reasoning given for this is that the dynamical fields in the theory vanish at spatial infinity. Although there may be instances in classical field theory where this boundary condition is applicable, generally this condition is too restrictive. Plane waves [89], or cases where the space of field configurations has a non-trivial topology [43], are two such examples where field solutions may not vanish asymptotically. In the quantum case, axiomatic formulations of field theory assert that fields φ are *operator-valued distributions* [49]. Distributions are continuous linear functionals which map a space of *test functions* $\mathcal{T}$ onto the complex numbers: $\varphi : \mathcal{T} \to \mathbb{C}$. In quantum field theory (QFT), $\mathcal{T}$ is chosen to be some set of space-time functions; usually either the space of continuous functions with compact support $\mathcal{D}(\mathbb{R}^{1,3})$, or the space of Schwartz functions[1] $\mathcal{S}(\mathbb{R}^{1,3})$. In either of these cases one can represent the image of the map φ on a space-time function f as:

$$\varphi(f) = (\varphi, f) := \int d^4x \; \varphi(x) f(x) \tag{2.1}$$

[1]The distributions with which these test functions are smeared are called *tempered distributions*.

which gives meaning to the x-dependent field expression $\varphi(x)$. Since φ is an *operator*-valued distribution in QFT, only the smeared expression $\varphi(f)$ is guaranteed to correspond to a well-defined operator. The derivative of a distribution φ' is defined by:

$$(\varphi', f) := -(\varphi, f') \tag{2.2}$$

and is itself also a distribution [49]. By applying the integral representation in Eq. (2.1), one can interpret this definition as an integration by parts where the boundary terms have been 'dropped':

$$\int d^4x \; \varphi'(x) f(x) = -\int d^4x \; \varphi(x) f'(x) \tag{2.3}$$

Although this shorthand notation is useful, and will be used for the calculations in this paper, it can also be slightly misleading. Sometimes it is incorrectly stated that integration by parts of quantum fields can be performed, and the boundary terms neglected. However, distributions are generally not point-wise defined, so boundary expressions like: $\int_{\partial\mathbb{R}^3} \varphi(x) f(x)$ are often ill-defined. Therefore, when manipulations like this are performed one is really just applying the definition of the derivative of a distribution, there are no boundary contributions. This makes the question of whether spatial boundary term operators vanish a more subtle issue in QFT than in the classical case.

The physical rationale behind using operator-valued distributions as opposed to operator-valued functions in QFT is because operators inherently imply a measurement, and this is not well-defined at a single (space-time) point since this would require an infinite amount of energy [50]. Instead, one can perform a measurement over a space-time region $\mathcal{U}$, and model the corresponding operator $\mathcal{A}(f)$ as a distribution $\mathcal{A}$ smeared with some test function f which has support in $\mathcal{U}$. If one were to smear $\mathcal{A}$ with another test function g, which has different support to f, then in general the operators $\mathcal{A}(f)$ and $\mathcal{A}(g)$ would be different. But the interpretation is that these operators measure the *same* quantity, just within the different space-time regions: $\mathrm{supp}(f)$ and $\mathrm{supp}(g)$.

As well as differentiation it is also possible to extend the notion of *multiplication by a function* to distributions. Given a distribution φ, a test function f, and some function g, this is defined as:

$$(g\varphi, f) := (\varphi, gf) \tag{2.4}$$

In order that $g\varphi$ defines a distribution in the case where $f \in \mathcal{D}$, it suffices that g be an infinitely differentiable function. For tempered distributions, in which $f \in \mathcal{S}$, it is also necessary that g and all of its derivatives are bounded by polynomials [49].

Besides the assumption that fields are operator-valued distributions, axiomatic approaches to QFT usually postulate several additional conditions that the theory must satisfy. Although different axiomatic schemes have been proposed, these schemes generally contain a common core set of axioms[2]. For the purpose of the calculations in this paper, the core axioms which play a direct role are:

1. **Local (anti-)commutativity**

   If the support of the test functions $f, g,$ *of the fields* $\Psi, \Phi,$ *are space-like separated then:*
   $$[\Psi(f), \Phi(g)]_{\pm} = \Psi(f)\Phi(g) \pm \Phi(g)\Psi(f) = 0$$
   holds when applied to any state vector, for any fields Ψ, Φ

2. **Non-degeneracy**

   The inner product $\langle\cdot|\cdot\rangle$ *on the space of states* $\mathcal{V}$ *is non-degenerate:*
   $$\langle\Psi|\omega\rangle = 0, \quad \forall|\Psi\rangle \in \mathcal{V} \quad \Longrightarrow \quad |\omega\rangle = 0$$

The physical motivation for the local (anti-)commutativity axiom is that it imposes a causality restriction on the theory. Since the action of field operators $\Psi(f)$ on states can be interpreted as the performance of a particular measurement in the space-time region $\mathrm{supp}(f)$ [50], if another measurement $\Phi(g)$ is performed in a space-time region $\mathrm{supp}(g)$ which is space-like separated to $\mathrm{supp}(f)$, the axiom states that these two measurements must either commute or anti-commute with one another. In physical terms this means that measurements which are performed a space-like distance apart cannot be causally related to one another. A space of fields $\mathcal{F}$ which satisfies this property is called a *local field algebra* [47]. By contrast, the non-degeneracy axiom can be imposed without any real loss of generality since any vector $|\omega\rangle$ whose inner product with any other state

[2] See [49–51] for a more in-depth discussion of these axioms and their physical motivation.

vanishes will not introduce physical effects into the theory that are describable using the inner product [51]. Such states $|\omega\rangle$ are therefore physically trivial with regards to the quantum theory, and can hence be set to zero.

Additional complications arise when defining quantised gauge field theories. This is because the restriction of a theory to be invariant under a gauge group symmetry $\mathcal{G}$, which corresponds to local invariance under some global symmetry group G, leads to a strengthened form of the Noether current conservation condition called the *local Gauss law* [47]:

$$J^a_\mu = \partial^\nu G^a_{\mu\nu}, \qquad G^a_{\mu\nu} = -G^a_{\nu\mu} \tag{2.5}$$

where J^a_μ is the Noether current associated with invariance under the global group G. Because of this condition it turns out that there are essentially two quantisation strategies [47]:

1. One demands that Eq. (2.5) holds as an operator equation, which implies that the algebra of fields $\mathcal{F}$ is no longer local. In particular, if a field transforms non-trivially with respect to the group G (i.e. has a non-zero G-charge), the field must be non-local.

2. One adopts a *local gauge quantisation* in which the local Gauss law is modified. This modification ensures that the field algebra remains local (even for charged fields), but necessitates the introduction of an indefinite inner product on the space of states $\mathcal{V}$, and a condition: $\langle\Psi|J^a_\mu - \partial^\nu G^a_{\mu\nu}|\Psi\rangle = 0$ for identifying the physical states $|\Psi\rangle \in \mathcal{V}_{\text{phys}} \subset \mathcal{V}$ (the *weak Gauss law*).

The advantage with the latter approach is that it allows one keep a local field algebra, and so all of the results from local field theory remain applicable. For the purposes of discussion in this paper we will only consider local quantisations, and in particular we will focus on the local BRST quantisation of Yang-Mills theory. A key feature of BRST quantisation is that a gauge-fixing term $\mathcal{L}_{GF}$ is added to the Lagrangian density $\mathcal{L}$. The modified Lagrangian $\mathcal{L}+\mathcal{L}_{GF}$ is no longer gauge-invariant, but remains invariant under a residual *BRST symmetry* with a conserved charge Q_B. By defining the physical space of states $\mathcal{V}_{\text{phys}} \subset \mathcal{V}$ to be the states which satisfy the *subsidiary* *condition*: $Q_B \mathcal{V}_{\text{phys}} = 0$, this ensures that the weak Gauss law is satisfied and that the field algebra $\mathcal{F}$ is local. The introduction of an indefinite inner product on $\mathcal{V}$ also leads to unphysical *negative* norm states, which are generated by the *Faddeev-Popov ghost* degrees of freedom in $\mathcal{L}_{GF}$. In terms of these extended state spaces, the physical Hilbert space is a quotient space of the form[3] $\mathcal{H} := \overline{\mathcal{V}_{\text{phys}}/\mathcal{V}_0}$, where $\mathcal{V}_0$ contains the zero norm states in $\mathcal{V}_{\text{phys}}$ [51].

The remainder of this paper is structured as follows; in Sec. 2.3 we apply these general QFT properties in order to establish a necessary and sufficient condition for spatial boundary terms to vanish, in Sec. 2.4 we give a theoretical overview of the angular momentum decomposition problem in QCD and why spatial boundary terms are of particular relevance, and in Sec. 2.5 we apply the results of Sec. 2.3 to this problem. Finally, in Sec. 2.6 we summarise our results and discuss their interpretation.

2.3 Spatial boundary terms in QFT

The aim of this section will be to demonstrate that the general properties of a quantum field theory, some of which were outlined in Sec. 2.2, are enough to establish a necessary and sufficient condition for spatial boundary terms of the form: $\int d^3x \; \partial_i B^i$ to vanish in the Hilbert space of physical states $\mathcal{H}$ [51], where $B^i(x)$ is some arbitrary local[4] field. However, before fully discussing this condition it is important to first outline the differences between the classical and quantum field theory approaches to conserved (and non-conserved) charges. Classically, charges Q are defined to be the spatial integral of the temporal component of some (not necessarily conserved) current density $j^\mu(x)$:

$$Q = \int d^3x \; j^0(x) \tag{2.6}$$

[3] The bar denotes the completion of $\mathcal{V}_{\text{phys}}/\mathcal{V}_0$ to include the limiting states of Cauchy sequences in $\mathcal{V}_{\text{phys}}/\mathcal{V}_0$.

[4] At least with gauge theories, no generality is lost by imposing locality since a local field algebra can always be assumed by adopting a local gauge quantisation [47].

However, in QFT $j^\mu(x)$ is typically some product of fields, and is therefore an operator-valued distribution[5]. This means that because no smearing with a test function has been performed, the quantised version of the classically motivated definition in Eq. (2.6) will generally *not* correspond to a proper operator in QFT [47]. But given some space-time test function f, a well-defined quantum representation of Q can be written:

$$Q = \int d^4x \; f(x) j^0(x) = j^0(f) \tag{2.7}$$

Following the discussion in Sec. 2.2, Q is interpreted as acting on the space-time region $\mathrm{supp}(f)$. In order to extend the action of Q to the whole of space, by analogy with the classical case, one can choose the following test function[6]: $f := \alpha(x_0) f_R(\mathbf{x})$, with $\alpha \in \mathcal{D}(\mathbb{R})$ ($\mathrm{supp}\,(\alpha) \subset [-\delta, \delta]$, $\delta > 0$) and $f_R \in \mathcal{D}(\mathbb{R}^3)$ where:

$$\int dx_0 \; \alpha(x_0) = 1, \qquad f_R(\mathbf{x}) = \begin{cases} 1, & |\mathbf{x}| < R \\ 0, & |\mathbf{x}| > R(1+\varepsilon) \end{cases} \tag{2.8}$$

with $\varepsilon > 0$. Because of the way f_R is defined this means that $\partial_i f_R$ vanishes for $|\mathbf{x}| < R$. Using these test functions one can then construct the following well-defined (localised) charge operator Q_R:

$$Q_R = \int d^4x \; \alpha(x_0) f_R(\mathbf{x}) j^0(x) \tag{2.9}$$

The reason why α and f_R are chosen to have this form is so that in the special case where the quantised version of the charge is genuinely conserved, this definition is in agreement with the classically-motivated form of Q (Eq. (2.6)) in the limit $R \to \infty$.

Setting: $j^0 = \partial_i B^i$ it is clear that spatial boundary terms: $\int d^3x \; \partial_i B^i$ are simply a special class of charges. Therefore, when: $\int d^3x \; \partial_i B^i$ is written in the proceeding discussion (for brevity), this actually corresponds to the smeared expression: $\lim_{R\to\infty} \int d^4x \; \alpha(x_0) f_R(\mathbf{x}) \partial_i B^i(x)$. With this notation in mind, one has the following theorem:

Theorem 1. $\int d^3x \; \partial_i B^i$ *vanishes in* $\mathcal{H}$ $\iff$ $\int d^3x \; \partial_i B^i |0\rangle = 0$

[5] Generally the product of distributions is not well-defined, and so one must first introduce a regularisation procedure in order to make sense of such products [50].

[6] This is the standard choice of test function chosen in the literature ([47, 51, 98, 99]) to define charges.

Proof ($\Longleftarrow$)**:** Let $\varphi \in \mathcal{F}(\mathcal{O})$ be some (smeared) local operator[7] and let $\alpha \in \mathcal{D}(\mathbb{R})$ and $f_R \in \mathcal{D}(\mathbb{R}^3)$ be the test functions of compact support defined in Eq. (2.8). Then:

$$\begin{aligned}\int d^3x \left(\partial_i B^i\right) \varphi|0\rangle &= \int d^3x \ \left[\partial_i B^i, \varphi\right]_{\pm} |0\rangle \\ &= \lim_{R\to\infty} \int d^4x \ \alpha(x_0) f_R(\mathbf{x}) \left[\partial_i B^i(x), \varphi\right]_{\pm} |0\rangle \\ &= -\lim_{R\to\infty} \int d^4x \ \alpha(x_0)(\partial_i f_R(\mathbf{x})) \left[B^i(x), \varphi\right]_{\pm} |0\rangle\end{aligned}$$

where in the first line one uses the assumption that: $\int d^3x \ \partial_i B^i|0\rangle = 0$ (with $|0\rangle$ the vacuum state), and in the last line the definition for the derivative of a distribution is used. Now because of the way f_R is defined it follows that: $\text{supp}\,(\partial_i f_R) = \{x \in \mathbb{R}^3;\ R \leq |\mathbf{x}| \leq R(1+\varepsilon)\}$, and so the support of $\alpha\partial_i f_R$ will be restricted to the space-time points: $(x_0, \mathbf{x})$, where $|\mathbf{x}| \geq R$ and $|x_0| \leq \delta$. So in the limit[8] $R \to \infty$ the supports of $\alpha\partial_i f_R$, and the test function for which φ is implicitly smeared, will become space-like separated. But by the local (anti-)commutativity axiom this implies that the (anti-)commutator in the last line must vanish exactly, and therefore: $\int d^3x \left(\partial_i B^i\right) \varphi|0\rangle = 0$. The vanishing of the (anti-)commutator is independent of the explicit form for α because α is continuous, has compact support, and is therefore bounded, which means that $\alpha\partial_i f_R$ will vanish wherever $\partial_i f_R$ does. Moreover, it follows directly from local (anti-)commutativity that the vanishing of the (anti-)commutator is also independent of the explicit form of f_R [99]. Because of the vanishing of: $\int d^3x \left(\partial_i B^i\right) \varphi|0\rangle$, one has:

$$\langle\Psi| \int d^3x \ \partial_i B^i(\varphi|0\rangle) = 0, \quad \forall|\Psi\rangle \in \mathcal{H}$$

and applying the *Reeh-Schlieder Theorem*[9] implies:

$$\langle\Psi| \int d^3x \ \partial_i B^i|\Phi\rangle = 0, \quad \forall|\Psi\rangle, |\Phi\rangle \in \mathcal{H}$$

which is precisely the statement that the spatial boundary term: $\int d^3x \ \partial_i B^i$ vanishes in $\mathcal{H}$. □

[7] $\mathcal{F}(\mathcal{O})$ is the polynomial algebra generated by field operators smeared with test functions with compact support in the bounded space-time region $\mathcal{O}$.

[8] The existence of this limit is guaranteed by the locality of B^i and φ [47].

[9] The Reeh-Schlieder Theorem implies that $\mathcal{H} = \overline{\mathcal{F}(\mathcal{O})|0\rangle}$ for any bounded open set $\mathcal{O}$, where the closure is with respect to some suitable topology. See [51] for a proof and in-depth discussion of this theorem.

Proof ($\Longrightarrow$)**:** Conversely, if one assumes that the spatial boundary term vanishes in $\mathcal{H}$ then:

$$\langle\Psi|\int d^3x\ \partial_i B^i|0\rangle = 0, \quad \forall|\Psi\rangle \in \mathcal{H}$$

since $|0\rangle \in \mathcal{H}$. But this inner product between states is taken to be non-degenerate, so the above condition implies that: $\int d^3x\ \partial_i B^i|0\rangle = 0$.

$\square$

One subtlety in establishing Theorem 1 comes from a property which is well-established in Quantum Electrodynamics (QED) [79], as well as other gauge theories [100] – *charged states are non-local*. This means that it is not possible to create a charged state by applying a *local* operator to the vacuum. However, by virtue of the Reeh-Schlieder Theorem, a charged state can always be approximated by local states as closely as one likes in the sense of convergence in some allowed topology on $\mathcal{H}$. Often this topology is chosen to be the *weak topology*[10] and so convergence means *weak convergence*. Therefore, given that $|\Phi\rangle \in \mathcal{H}$ is a charged state, there exists a sequence of *local* operators $\{\varphi_n\}$ such that $\lim_{n\to\infty}\langle\Psi|\varphi_n|0\rangle = \langle\Psi|\Phi\rangle,\ \forall|\Psi\rangle \in \mathcal{H}$. In QED it has in fact been explicitly shown that physical charged states can be constructed from weak limits of local states [101]. With this convergence property in mind, the proof of Theorem 1 can then still be shown to hold in the case where $|\Phi\rangle$ is a charged state, since one can apply the same steps as before with φ replaced by φ_n, conclude that: $\langle\Psi|\int d^3x\ \partial_i B^i(\varphi_n|0\rangle) = 0,\ \forall|\Psi\rangle \in \mathcal{H}$, and then take the limit $n \to \infty$. Moreover, because the (anti-)commutator in the proof is shown to vanish regardless of the explicit form of both α and f_R, this demonstrates that Theorem 1 holds independently of the specific test functions in the smearing, and can hence be applied to all spatial boundary term operators of the form: $\int d^3x\ \partial_i B^i$, where $B^i(x)$ is any local field.

The proof of Theorem 1 is based on similar discussions in [47, 51, 98, 99], which address the issue of defining a consistent local charge operator and its action on states in $\mathcal{H}$. The surprising conclusion of this theorem is that the vanishing of a spatial boundary

[10] Generally it is desirable that the Hilbert space topology be an *admissible topology*, which means that the continuity of a linear functional ℓ on $\mathcal{H}$ is equivalent to the existence of a vector $|\Phi\rangle \in \mathcal{H}$ such that: $\ell\left(|\Psi\rangle\right) = \langle\Phi|\Psi\rangle$. The weakest admissible topology is the weak topology [51].

term only requires that the corresponding operator annihilates the vacuum state – *it is independent of how this operator acts on the full space of states.* This result has interesting physical consequences for any QFT, but in particular its relevance to the angular momentum decomposition problem in Quantum Chromodynamics (QCD) will be discussed in Secs. 2.4 and 2.5.

Generally, Theorem 1 demonstrates that a spatial boundary term operator annihilating the vacuum state is both a necessary and a sufficient condition for that boundary term itself to vanish in the physical Hilbert space $\mathcal{H}$. However, in order to practically determine whether this operator annihilates the vacuum or not, it is easier to instead relate these conditions to equivalent conditions involving matrix elements. This connection is given by the following simple relations:

$$\text{If } \langle\Psi|\int d^3x\ \partial_i B^i|0\rangle = 0,\ \forall|\Psi\rangle\in\mathcal{H} \implies \int d^3x\ \partial_i B^i|0\rangle = 0 \tag{2.10}$$

$$\text{If } \exists|\Psi\rangle\in\mathcal{H} \text{ s.t. } \langle\Psi|\int d^3x\ \partial_i B^i|0\rangle \neq 0 \implies \int d^3x\ \partial_i B^i|0\rangle \neq 0 \tag{2.11}$$

Eq. (2.10) follows immediately from the assumption that the inner product in $\mathcal{H}$ is non-degenerate, and Eq. (2.11) is the logical negation of the statement that the boundary operator acting on the vacuum state is the null vector in $\mathcal{H}$. These relations imply that if one can find *any* state $|\Psi\rangle \in \mathcal{H}$ such that: $\langle\Psi|\int d^3x\ \partial_i B^i|0\rangle \neq 0$, then this definitively proves: $\int d^3x\ \partial_i B^i|0\rangle \neq 0$, and hence by Theorem 1 that: $\int d^3x\ \partial_i B^i \neq 0$. Otherwise, it must be the case that: $\int d^3x\ \partial_i B^i|0\rangle = 0$, and thus: $\int d^3x\ \partial_i B^i = 0$. To determine the explicit form of these matrix elements one can use the transformation property of fields under translations [50]:

$$B^i(x) = e^{iP_\mu x^\mu} B^i(0) e^{-iP_\mu x^\mu} \tag{2.12}$$

and insert this between the states $|\Psi\rangle$ and $|0\rangle$ to obtain:

$$\begin{aligned}\langle\Psi|\int d^3x\ \partial_i\Big[e^{iP_\mu x^\mu}B^i(0)e^{-iP_\mu x^\mu}\Big]|0\rangle &= \langle\Psi|\int d^3x\ \Big[(iP_i)e^{iP_\mu x^\mu}B^i(0)e^{-iP_\mu x^\mu} \\ &\qquad + e^{iP_\mu x^\mu}B^i(0)e^{-iP_\mu x^\mu}(-iP_i)\Big]|0\rangle \\ &= \langle\Psi|\int d^3x\ \Big[(iP_i)e^{iP_\mu x^\mu}B^i(0)\Big]|0\rangle\end{aligned}$$

where the second term in the first line vanishes because $P_\mu|0\rangle = 0$. Now if one takes

$|\Psi\rangle$ to be some momentum eigenstate $|p\rangle$, the above relation simplifies to:

$$\langle p| \int d^3x \; \partial_i B^i |0\rangle = \begin{cases} 0, & p = 0 \\ \lim_{R\to\infty} \int d^4x \; ip_i \alpha(x_0) f_R(\mathbf{x}) e^{ip_\mu x^\mu} \langle p|B^i(0)|0\rangle, & p \neq 0 \end{cases} \tag{2.13}$$

It is interesting to note here that the vacuum expectation value of the spatial boundary operator: $\int d^3x \; \partial_i B^i$ completely vanishes, whereas the off-diagonal matrix element depends on the local term: $\langle p|B^i(0)|0\rangle$.

2.4 The proton angular momentum decomposition

Theoretical investigations into the spin structure of nucleons have been ongoing ever since the inception of QCD in the 1960s. The evolution of this research area has been influenced by a number of different experimental groups including the European Muon Collaboration (EMC), the Spin Muon Collaboration, and more recently HERMES, COMPASS, STAR and PHENIX [89]. The focal point of these investigations have largely centred around settling an unresolved dispute known as the *spin crisis*, which refers to results obtained by the EMC experiment [90] that suggested quarks accounted for 'only' a very small amount of the spin of the proton. Many of the proposed solutions to the spin crisis are based on splitting the QCD angular momentum operator up in different ways, and then arguing a particular physical interpretation of the resulting pieces. It turns out that spatial boundary terms play a prominent role in these decompositions. More specifically, during the rest of this section we will outline why the vanishing of certain spatial boundary *superpotential* terms is an essential assumption in this analysis.

As discussed in Sec. 2.2, in order to analyse the dynamical properties of quantised Yang-Mills theory (in this case QCD), one must choose a quantisation procedure. For the analysis in this paper we will consider the local BRST quantisation with the following

Hermitian, gauge-fixed Lagrangian density as proposed by [98]:

$$\mathcal{L}_{QCD} = -\frac{1}{4}F^a_{\mu\nu}F^{\mu\nu a} + \overline{\psi}\left(\frac{i}{2}\gamma^\mu(\overrightarrow{\partial}_\mu - \overleftarrow{\partial}_\mu) + gT^a A^a_\mu\gamma^\mu - m\right)\psi + \mathcal{L}_{GF} + \mathcal{L}_{FP} \quad (2.14)$$

$$\mathcal{L}_{GF} = -(\partial^\mu B^a)A^a_\mu + \frac{\xi}{2}B^a B^a \quad (2.15)$$

$$\mathcal{L}_{FP} = -i\partial^\mu \overline{C}^a (D_\mu C)^a \quad (2.16)$$

where $C^a, \overline{C}^a$ are the Faddeev-Popov ghost fields, B^a is the auxiliary gauge fixing field, ξ is a gauge fixing parameter, and one defines: $(D_\mu C)^a := \partial_\mu C^a - gf^{abc}A^c_\mu C^b$. To determine the spin structure of QCD one must first define the energy-momentum tensor of the theory $T^{\mu\nu}_{QCD}$. As with any current density the definition of $T^{\mu\nu}$ is always ambiguous up to a sign, but for the purposes of this paper the following definition will be used:

$$T^{\mu\nu} = \frac{2}{\sqrt{-g}}\frac{\delta S}{\delta g_{\mu\nu}} \quad (2.17)$$

where: $g = \det g_{\mu\nu}$, $S = \int d^4x\sqrt{-g}\,\mathcal{L}$, and $\mathcal{L}$ has the formal functional dependence: $\mathcal{L} = \mathcal{L}(g_{\mu\nu}, \Psi^I, \nabla_\alpha \Psi^I)$, with ∇_α the general relativistic covariant derivative[11] and $\{\Psi^I\}$ the dynamical fields in the theory (with possible internal index I). As was famously shown by Belinfante [93], this expression can always be decomposed into the following form:

$$T^{\mu\nu} = T^{\mu\nu}_c + \frac{1}{2}\partial_\rho\left(S^{\rho\mu\nu} + S^{\mu\nu\rho} + S^{\nu\mu\rho}\right) \quad (2.18)$$

where $T^{\mu\nu}_c$ is the canonical energy-momentum tensor and $S^{\rho\mu\nu}$ is the so-called spin-angular momentum density term [51]:

$$T^{\mu\nu}_c := \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Psi^I)}\partial^\nu\Psi^I - g^{\mu\nu}\mathcal{L}, \qquad S^{\rho\mu\nu} := -i\frac{\partial\mathcal{L}}{\partial(\partial_\rho\Psi^I)}(s^{\mu\nu})^I_J\Psi^J \quad (2.19)$$

$(s^{\mu\nu})^I_J$ corresponds to the Lorentz generator $s^{\mu\nu}$ in the finite-dimensional representation[12] of the field Ψ^I. It is interesting to note that the question of whether the quantised Belinfante or canonical energy-momentum tensor is physically more relevant is still an on-going issue [89]. A discussion of the related subtleties between the Belinfante P^μ

[11] $\nabla_\alpha\Psi^I$ varies in form depending on the type of field Ψ^I

[12] E.g. for a vector field: $(s^{\mu\nu}_V)^I_J = i(g^{\mu I}\delta^\nu{}_J - g^{\nu I}\delta^\mu{}_J)$, where I, J are space-time indices, whereas for a spinor field: $(s^{\mu\nu}_S)^I_J = \frac{i}{4}[\gamma^\mu,\gamma^\nu]^I_J$, with I, J spinor indices.

and canonical P_c^μ momentum operators is given in 2.7. Applying the definition in Eq. (2.18) to QCD, one obtains the following expression for the energy-momentum tensor [98]:

$$T^{\mu\nu}_{QCD} = T^{\mu\nu}_{\text{phys}} - \left\{ Q_B,\ (\partial^\mu \overline{C}^a) A^{\nu a} + (\partial^\nu \overline{C}^a) A^{\mu a} + g^{\mu\nu} \left(\frac{1}{2} \xi \overline{C}^a B^a - (\partial^\rho \overline{C}^a) A^a_\rho \right) \right\} \tag{2.20}$$

$$T^{\mu\nu}_{\text{phys}} = \frac{1}{2} \overline{\psi} \left(\frac{i}{2} \gamma^\mu (\overrightarrow{\partial^\nu} - \overleftarrow{\partial^\nu}) + g T^a A^{\nu a} \gamma^\mu \right) \psi + \ (\mu \leftrightarrow \nu) + F^{\mu a}_{\ \ \rho} F^{\rho\nu a} + \frac{1}{4} g^{\mu\nu} F^a_{\alpha\beta} F^{\alpha\beta a} \tag{2.21}$$

where Q_B is the BRST charge. In any field theory the current associated with Lorentz transformations is the rank-3 tensor defined by [93]:

$$M^{\mu\nu\lambda} := x^\nu T^{\mu\lambda} - x^\lambda T^{\mu\nu} \tag{2.22}$$

Using this definition, the Lorentz current in QCD can be written:

$$\begin{aligned} M^{\mu\nu\lambda}_{QCD} = x^\nu T^{\mu\lambda}_{\text{phys}} - x^\lambda T^{\mu\nu}_{\text{phys}} + i x^{[\nu} \delta_B \Big[& (\partial^\mu \overline{C}^a) A^{\lambda]a} + (\partial^{\lambda]} \overline{C}^a) A^{\mu a} \\ & + g^{\mu\lambda]} \left(\frac{1}{2} \xi \overline{C}^a B^a - (\partial^\rho \overline{C}^a) A^a_\rho \right) \Big] \end{aligned}$$

where $\delta_B : \mathcal{F} \to \mathcal{F}$ is the BRST variation map defined for $\mathcal{R} \in \mathcal{F}$ by:

$$\delta_B \mathcal{R} := [i Q_B, \mathcal{R}]_\pm \tag{2.23}$$

and $\pm$ signifies an anti-commutator or commutator depending on whether $\mathcal{R}$ has an odd or an even *ghost number*[13] respectively. The remarkable thing about this structure is that all of the ghost and gauge fixing fields are contained in a single BRST variation (coboundary) term, and this guarantees that these unphysical operators will not contribute[14] to any physical matrix element involving states in $\mathcal{H}$ [51]. For this reason we will not discuss this term any longer and will simply set: $T^{\mu\nu}_{QCD} \equiv T^{\mu\nu}_{\text{phys}}$. The remaining

[13]The ghost number corresponds to the number of ghost fields contained in a composite operator [51].

[14]Nevertheless, these unphysical fields are still essential for ensuring the consistency and Lorentz covariance of the theory.

physical QCD Lorentz current then takes the form:

$$
\begin{aligned}
M^{\mu\nu\lambda}_{QCD} &= x^{\nu}\Big[\frac{1}{2}\overline{\psi}\left(\frac{i}{2}\gamma^{\mu}(\overrightarrow{\partial^{\lambda}} - \overleftarrow{\partial^{\lambda}}) + gT^{a}A^{\lambda a}\gamma^{\mu}\right)\psi + \ (\mu \leftrightarrow \lambda) + F^{\mu a}_{\ \ \rho}F^{\rho\lambda a} + \frac{1}{4}g^{\mu\lambda}F^{a}_{\alpha\beta}F^{\alpha\beta a}\Big] \\
&\quad - x^{\lambda}\Big[\frac{1}{2}\overline{\psi}\left(\frac{i}{2}\gamma^{\mu}(\overrightarrow{\partial^{\nu}} - \overleftarrow{\partial^{\nu}}) + gT^{a}A^{\nu a}\gamma^{\mu}\right)\psi + \ (\mu \leftrightarrow \nu) + F^{\mu a}_{\ \ \rho}F^{\rho\nu a} + \frac{1}{4}g^{\mu\nu}F^{a}_{\alpha\beta}F^{\alpha\beta a}\Big] \\
&= x^{\nu}F^{\mu a}_{\ \ \rho}F^{\rho\lambda a} - x^{\lambda}F^{\mu a}_{\ \ \rho}F^{\rho\nu a} + \frac{1}{4}F^{a}_{\alpha\beta}F^{\alpha\beta a}(x^{\nu}g^{\mu\lambda} - x^{\lambda}g^{\mu\nu}) \\
&\quad + \frac{i}{4}\Big[x^{\nu}\overline{\psi}(\gamma^{\mu}D^{\lambda} + \gamma^{\lambda}D^{\mu})\psi - (\nu \leftrightarrow \lambda)\Big] + \ \text{h.c.}
\end{aligned}
\tag{2.24}
$$

where $D^{\mu} := \partial^{\mu} - igT^{a}A^{\mu a}$ is the covariant derivative and h.c. denotes the Hermitian conjugate. Individually, the terms in Eq. (2.24) do not have a clear interpretation. However, in the early discussion of $M^{\mu\nu\lambda}_{QCD}$ in the literature it was suggested [81] that a more meaningful expression can be obtained by factoring out total divergence terms. In this case it turns out that one can write [81]:

$$
\begin{aligned}
M^{\mu\nu\lambda}_{QCD} =& \frac{i}{2}\overline{\psi}\gamma^{\mu}\left(x^{\nu}\partial^{\lambda} - x^{\lambda}\partial^{\nu}\right)\psi + \ \text{h.c.} \ + \frac{1}{2}\epsilon^{\mu\nu\lambda\rho}\overline{\psi}\gamma_{\rho}\gamma^{5}\psi \\
&- F^{\mu\rho a}\left(x^{\nu}\partial^{\lambda} - x^{\lambda}\partial^{\nu}\right)A^{a}_{\rho} + F^{\mu\lambda a}A^{\nu a} + F^{\nu\mu a}A^{\lambda a} + \frac{1}{4}F^{a}_{\alpha\beta}F^{\alpha\beta a}\left(x^{\nu}g^{\mu\lambda} - x^{\lambda}g^{\mu\nu}\right) \\
&- \frac{i}{16}\partial_{\beta}\Big[x^{\nu}\overline{\psi}\{\gamma^{\lambda},[\gamma^{\mu},\gamma^{\beta}]\}\psi - (\nu \leftrightarrow \lambda)\Big] + \partial_{\beta}(x^{\nu}F^{\mu\beta a}A^{\lambda a} - x^{\lambda}F^{\mu\beta a}A^{\nu a})
\end{aligned}
\tag{2.25}
$$

If one then *chooses* to drop these divergence terms, the current takes the following partitioned form:

$$
\begin{aligned}
M^{\mu\nu\lambda}_{QCD} =& \frac{i}{2}\overline{\psi}\gamma^{\mu}\left(x^{\nu}\partial^{\lambda} - x^{\lambda}\partial^{\nu}\right)\psi + \ \text{h.c} \ + \frac{1}{2}\epsilon^{\mu\nu\lambda\rho}\overline{\psi}\gamma_{\rho}\gamma^{5}\psi \\
&- F^{\mu\rho a}\left(x^{\nu}\partial^{\lambda} - x^{\lambda}\partial^{\nu}\right)A^{a}_{\rho} + F^{\mu\lambda a}A^{\nu a} + F^{\nu\mu a}A^{\lambda a} + \frac{1}{4}F^{a}_{\alpha\beta}F^{\alpha\beta a}\left(x^{\nu}g^{\mu\lambda} - x^{\lambda}g^{\mu\nu}\right)
\end{aligned}
\tag{2.26}
$$

This is often referred to in the literature as the *Jaffe-Manohar decomposition* [88, 89]. The fundamental difference between this expression and the expression in Eq. (2.24) is that the interaction terms between the quark and gluon fields do not feature[15], and this makes it easier to give the individual remaining terms a physical interpretation. It also turns out that one can arrive at this same decomposition by instead using the canonical

[15]The gluon self-interaction terms do still feature in the expression though.

energy-momentum tensor $T_c^{\mu\nu}$, and in this context this is referred to as the canonical version of the Lorentz current [89]. In a similar manner to the above derivation, it is also necessary in this case to drop certain divergence terms in order to arrive at the decomposition in Eq. (2.26). By applying the definition for the angular momentum charge:

$$J^i_{QCD} := \frac{1}{2}\, \epsilon^{ijk} \int d^3x \; M^{0jk}_{QCD}(x) \tag{2.27}$$

the decomposition of the current in Eq. (2.26) becomes a decomposition of charges. These charges are often then individually interpreted as corresponding to physically distinct angular momentum sources [82–86]. As well as the Jaffe-Manohar decomposition there also exist many other possible ways of decomposing J^i_{QCD} [85, 89]. Despite the variety in structure of these different decompositions, it turns out [89] that they all differ from one another by terms of the form: $\partial_\beta B^{[\mu\beta][\nu\lambda]}$, which are called *superpotentials*[16] [81]. Therefore, in order for any of these decompositions to hold one is required to drop superpotential terms, and if this procedure is justified it implies that all of the possible decompositions are physically equivalent to one another [89].

The argument in the literature [81] for dropping superpotential terms goes as follows: if two current densities $\widetilde{M}$ and M differ by a superpotential:

$$\widetilde{M}^{\mu\nu\lambda} = M^{\mu\nu\lambda} + \partial_\beta B^{[\mu\beta][\nu\lambda]}$$

then the corresponding charges $\widetilde{J}^{\nu\lambda} = \int d^3x \; \widetilde{M}^{0\nu\lambda}$ and $J^{\nu\lambda} = \int d^3x \; M^{0\nu\lambda}$ must be related by:

$$\widetilde{J}^{\nu\lambda} = J^{\nu\lambda} + \int d^3x \, \partial_i B^{[0i][\nu\lambda]}$$

Assuming that $B^{[0i][\nu\lambda]}(x)$ vanishes at spatial infinity, the divergence theorem implies that: $\widetilde{J}^{\nu\lambda} = J^{\nu\lambda}$, and so for computing charges the currents $\widetilde{M}^{\mu\nu\lambda}$ and $M^{\mu\nu\lambda}$ are indistinguishable. However, the results and discussions in Secs. 2.2 and 2.3 demonstrate that this argument is often too simplistic in the classical case, and is also not transferable to the corresponding quantised theory. Nevertheless, these arguments for dropping boundary terms have been applied to many situations, one of which being the derivation of the *proton angular momentum sum rule* [81, 83]. This derivation starts

[16] The notation $B^{[\mu\beta][\nu\lambda]}$ implies that $B^{\mu\beta\nu\lambda}$ is anti-symmetric in the indices (μ, β) and (ν, λ).

by taking the full expression for $M^{\mu\nu\lambda}_{QCD}$ (Eq. (2.25)) and inserting it into Eq. (2.27), giving:

$$
\begin{aligned}
J^i_{QCD} = & \underbrace{\epsilon^{ijk}\int d^3x \left[\frac{i}{2}\overline{\psi}\gamma^0\left(x^j\partial^k\right)\psi + \text{ h.c.}\right]}_{:=L^i_q} + \underbrace{\epsilon^{ijk}\int d^3x \left[\frac{1}{4}\epsilon^{0jkl}\overline{\psi}\gamma_l\gamma^5\psi\right]}_{:=S^i_q} \\
& \underbrace{-\epsilon^{ijk}\int d^3x \left[F^{0la}\left(x^j\partial^k\right)A^a_l\right]}_{:=L^i_g} + \underbrace{\epsilon^{ijk}\int d^3x \left[F^{0ka}A^{ja}\right]}_{:=S^i_g} \\
& \underbrace{-\frac{i}{16}\epsilon^{ijk}\int d^3x\ \partial_l\Big[x^j\overline{\psi}\{\gamma^k,[\gamma^0,\gamma^l]\}\psi\Big]}_{:=\mathcal{S}^i_1} + \underbrace{\epsilon^{ijk}\int d^3x\ \partial_l(x^jF^{0la}A^{ka})}_{:=\mathcal{S}^i_2}
\end{aligned} \tag{2.28}
$$

If one then assumes that the superpotential boundary terms $\mathcal{S}^i_1$ and $\mathcal{S}^i_2$ in this expression vanish, and inserts the remaining z-components ($i = 3$) between z-polarised proton states[17] $|p,s\rangle$, one obtains the proton angular momentum sum rule [81, 83]:

$$
\frac{1}{2} = \frac{1}{2}\Sigma + L_q + S_g + L_g \tag{2.29}
$$

where the $\frac{1}{2}$ term on the left-hand side comes from the fact that: $J^3_{QCD}|p,s\rangle = \frac{1}{2}|p,s\rangle$, and each of the other terms are defined by:

$$
\frac{1}{2}\Sigma = \frac{\langle p,s|S^3_q|p,s\rangle}{\langle p,s|p,s\rangle}, \quad S_g = \frac{\langle p,s|S^3_g|p,s\rangle}{\langle p,s|p,s\rangle}, \quad L_q = \frac{\langle p,s|L^3_q|p,s\rangle}{\langle p,s|p,s\rangle}, \quad L_g = \frac{\langle p,s|L^3_g|p,s\rangle}{\langle p,s|p,s\rangle}
$$

where a sum over quark flavour is also implicitly assumed in the definitions of Σ and L_q. Σ/S_g are then interpreted as the contributions to the z-component of the internal spin of the proton from quarks/gluons[18], and L_q/L_g the contributions to the z-component of the orbital angular momentum of the proton from the quarks/gluons. It is clear that this derivation requires that the superpotential boundary terms either exactly vanish, or at least vanish when inserted between proton states. In the next section we will use the results of Sec. (2.3) to address whether either of these conditions is actually satisfied in this case.

[17] There are of course subtleties [47] in how to define such asymptotic states, but we will not discuss these here.

[18] The interpretation of Σ and S_g comes from the equality of these terms with the corresponding partonic quantities in the infinite momentum frame and $A^0 = 0$ gauge [81, 83].

2.5 Superpotential boundary terms in QCD

In this section we will focus on addressing the issue of angular momentum decompositions in QCD, and in particular whether the proton angular momentum sum rule holds. As discussed in Sec. (2.4), to tackle this question it is important to understand superpotential spatial boundary terms of the form: $\int d^3x\ \partial_i \left(x^j B^{k0i}\right)$, where $B^{k0i}(x)$ is local. Despite the explicit x-dependence, Theorem 1 continues to hold with the replacement: $B^i \to x^j B^{k0i}$ because the function multiplication property of distributions (Eq. (2.4)) allows one to re-write the boundary operator in terms of B^{k0i} smeared with the test function $x^j \alpha \partial_i f_R$, and so the local (anti-)commutativity argument continues to hold. In Sec. 2.4 it was established that in order for the derivation of the proton angular momentum sum rule to remain valid, it must be the case that either one of the following conditions is satisfied:

1. The superpotential boundary term operators $\mathcal{S}_1^i$ and $\mathcal{S}_2^i$ are exactly vanishing.
2. These operators vanish when inserted between identical z-polarised proton states $|p, s\rangle$.

Using the conditions in Eqs. (2.10) and (2.11) the first statement can be tested as follows:

$$\text{If } \exists |p\rangle \in \mathcal{H} \text{ s.t: } \langle p| \int d^3x\ \partial_i \left(x^j B^{k0i}(x)\right) |0\rangle \neq 0 \quad \Longrightarrow \quad \int d^3x\ \partial_i \left(x^j B^{k0i}(x)\right) \neq 0 \tag{2.30}$$

By performing an analogous calculation to the one at the end of Sec. 2.3, the matrix elements of the superpotential operator: $\int d^3x\ \partial_i \left(x^j B^{k0i}(x)\right)$ can be written in the form:

$$\langle p| \int d^3x\ \partial_i \left(x^j B^{k0i}(x)\right) |0\rangle = \begin{cases} \lim_{R\to\infty} \int d^3x\ f_R(\mathbf{x}) \langle 0| B^{k0j}(0)|0\rangle, & p = 0 \\ \lim_{R\to\infty} \int d^4x\ \alpha(x_0) f_R(\mathbf{x}) e^{ip_\mu x^\mu} \Big[\langle p| B^{k0j}(0)|0\rangle & \\ \qquad\qquad + ip_i \langle p| x^j B^{k0i}(0)|0\rangle\Big], & p \neq 0 \end{cases} \tag{2.31}$$

where $|p\rangle$ is some momentum eigenstate. In the case of the Jaffe-Manohar angular momentum decomposition discussed in Sec. 2.4, the superpotential boundary terms $\mathcal{S}_1^i$

and $\mathcal{S}_2^i$ are given by:

$$\mathcal{S}_1^i = -\frac{i}{16}\epsilon^{ijk}\int d^3x\ \partial_l\left(x^j\overline{\psi}\{\gamma^k,[\gamma^0,\gamma^l]\}\psi\right), \qquad \mathcal{S}_2^i = \epsilon^{ijk}\int d^3x\ \partial_l\left(x^jF^{0la}A^{ka}\right) \quad (2.32)$$

Choosing $|p\rangle = |0\rangle$, and applying Eq. (2.31), the matrix elements of these operators can then be written:

$$\langle 0|\mathcal{S}_1^i|0\rangle = \lim_{R\to\infty}\int d^3x\ \frac{1}{4}f_R(\mathbf{x})\epsilon^{ijk}\epsilon^{0jkl}\langle 0|\overline{\psi}\gamma^l\gamma^5\psi|0\rangle$$
$$\langle 0|\mathcal{S}_2^i|0\rangle = \lim_{R\to\infty}\int d^3x\ f_R(\mathbf{x})\epsilon^{ijk}\langle 0|F^{0ja}A^{ka}|0\rangle$$

In both cases these expressions are non-zero if the vacuum expectation values

$$\epsilon^{ijk}\epsilon^{0jkl}\langle 0|\overline{\psi}\gamma^l\gamma^5\psi|0\rangle, \qquad \epsilon^{ijk}\langle 0|F^{0ja}A^{ka}|0\rangle$$

are non-zero. It is important to note here that these expressions are non-trivial because the fields involved are solutions to the full interacting theory, and so their expectation values are non-perturbative objects. Moreover, these combinations of fields do not correspond to conserved currents, so one cannot infer their value based on conservation properties. In order to establish the value of expressions such as these one must either employ a non-perturbative technique (such as lattice gauge theory), or make use of additional symmetries to restrict their form. Calculations such as these have been performed in the literature, and there is evidence to suggest that the first of these vacuum expectation values is non-vanishing [102]. The second expression though has not to our knowledge been computed[19]. In the special case where one takes: $|\Psi\rangle = |\pi\rangle$ (the pion state) for the expectation value in the first case, then one can use the hypothesised relation:

$$\langle\pi|\overline{\psi}\gamma^l\gamma^5\psi|0\rangle = if_\pi p^l \quad (2.33)$$

where $f_\pi \neq 0$ is the *pion form factor* [104] and p^l is the pion's 3-momentum. Inserting this expression into Eq. (2.31) also gives a non-zero result for the $p \neq 0$ case. Applying the condition in Eq. (2.30), these results suggest that $\mathcal{S}_1^i$ is in general non-vanishing. Therefore, since $\mathcal{S}_2^i$ does not cancel $\mathcal{S}_1^i$, this casts doubt on the validity of the angular momentum operator decomposition: $J^i_{QCD} = S^i_q + L^i_q + S^i_g + L^i_g$.

[19] The similar expression $\langle A^2\rangle$ has been computed though, using lattice QCD, and was found to be non-zero [103].

To compute whether condition 2 is satisfied or not one must calculate the matrix elements of the superpotential operators $\mathcal{S}_1^i$ and $\mathcal{S}_2^i$ between the z-polarised proton states $|p,z\rangle$. Performing this calculation one obtains:

$$\begin{aligned}
\langle p,s|\mathcal{S}_1^i|p,s\rangle &= \lim_{R\to\infty}\int d^3x\ \frac{1}{4}f_R(\mathbf{x})\epsilon^{ijk}\epsilon^{0jkl}\langle p,s|\overline{\psi}\gamma^l\gamma^5\psi|p,s\rangle \\
\langle p,s|\mathcal{S}_2^i|p,s\rangle &= \lim_{R\to\infty}\int d^3x\ f_R(\mathbf{x})\epsilon^{ijk}\langle p,s|F^{0ja}A^{ka}|p,s\rangle
\end{aligned}$$

Without applying a non-perturbative technique it is unclear whether either of these expressions are vanishing or not. However, by computing the same matrix elements for the operators S_q^i and S_g^i in Eq. (2.28), it turns out that the following exact relations hold:

$$\langle p,s|S_q^i|p,s\rangle = -\langle p,s|\mathcal{S}_1^i|p,s\rangle \tag{2.34}$$

$$\langle p,s|S_g^i|p,s\rangle = -\langle p,s|\mathcal{S}_2^i|p,s\rangle \tag{2.35}$$

This means that regardless of whether these terms vanish or not, the proton matrix elements for $\mathcal{S}_1^i$ and $\mathcal{S}_2^i$ will actually cancel the corresponding matrix elements for the 'spin' operators S_q^i and S_g^i in the angular momentum sum rule. The physical interpretation of the sum rule is therefore lost, and so L_q/L_g can no longer be interpreted as orbital angular momentum observables. It is also clear that the matrix elements Σ and S_g are not constrained since they do not contribute to the sum rule. A similar cancellation to Eq. (2.34) was also found in [105], although this approach relied on a wave-packet and form factor formulation which was later shown by [106] to not hold in general.

The analysis in this section demonstrates that neither conditions 1 nor 2 are satisfied, and therefore the validity of the derivation of the angular momentum sum rule is undermined. Physically speaking, it is the non-perturbative structure of QCD which prevents one from forming distinct quark and gluon observables in this way. These results also provide a resolution to the spin crisis since the cancellation of the Σ term in the sum rule lifts the constraint on Σ, which means that there is no longer an a priori expectation as to what value this matrix element should take.

2.6 Conclusions

Spatial boundary term operators play an important role in quantum field theories, and in particular the issue of whether they vanish or not is a recurring theme in many of the applications of these theories. The main aim of this paper was to use an axiomatic field theory approach in order to establish a concrete condition on when these terms vanish. It turns out that a necessary and sufficient condition for this class of operators to vanish is that the operator must annihilate the vacuum state. This is a somewhat surprising result in itself because it is completely independent of how this operator acts on the full space of states. In the remainder of this paper we applied this result in order to address the issue of whether meaningful quark-gluon angular momentum operator decompositions are possible in QCD. It turns out that a common feature of these decompositions is the necessity to drop certain spatial boundary terms called *superpotentials*. Using the boundary term conditions established in the previous part of the paper, we analysed the superpotential terms for the specific case of the *Jaffe-Manohar decomposition* derived from the Belinfante energy-momentum tensor, with the conclusion that the sum of these superpotential operators is non-vanishing. In this context, this suggests that the Jaffe-Manohar angular momentum operator decomposition does not hold. An important consequence of these non-trivial boundary operators is the effect that they have on the *proton angular momentum sum rule*. By keeping these boundary terms explicit, we found that the sum rule is modified in a rather surprising way – the supposed gluon S_g and quark Σ spin terms are completely cancelled in the expression. This throws into doubt the physical interpretation of these terms and also provides a resolution to the proton spin crisis, since the cancellation of the Σ term in the sum rule lifts the constraint on Σ, and therefore one loses any expectation on what value it should take. Physically speaking, the boundary term conditions imply that the non-perturbative structure of QCD prevents the possibility of forming distinct quark and gluon observables in this way.

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2.7 Appendix

Because of the way the Belinfante energy-momentum tensor is defined in Eq. (2.18), the Belinfante P^μ and canonical P_c^μ momentum operators are related to one another as follows:

$$P^\mu = P_c^\mu + \int d^3x \; \partial_i B^{i\mu} \tag{2.36}$$

where $B^{i\mu} = \frac{1}{2}\left(S^{i0\mu} + S^{0\mu i} + S^{\mu 0i}\right)$. So P^μ and P_c^μ differ by a spatial boundary term. Since P_c^μ is the generator of translations this means that: $[iP_c^\mu, F(y)] = \partial^\mu F(y)$, where $F(y)$ is any local field. However, because of the relation in Eq. (2.36), it follows that:

$$\begin{aligned}
[iP^\mu, F(y)] &= [iP_c^\mu, F(y)] + i\int d^3x \; [\partial_i B^{i\mu}, F(y)] \\
&= [iP_c^\mu, F(y)] + i\lim_{R\to\infty}\int d^4x \; \alpha(x_0) f_R(\mathbf{x})\left[\partial_i B^{i\mu}(x), F(y)\right] \\
&= [iP_c^\mu, F(y)] - \underbrace{i\lim_{R\to\infty}\int d^4x \; \alpha(x_0)\left(\partial_i f_R(\mathbf{x})\right)\left[B^{i\mu}(x), F(y)\right]}_{=0} \\
&= \partial^\mu F(y)
\end{aligned}$$

where the second term in the penultimate line vanishes by exactly the same local (anti-)commutativity argument as used in the proof of Theorem 1 in Sec. 2.3. So the Belinfante momentum operator P^μ is *also* a generator of space-time translations. Nevertheless, P^μ and P_c^μ may well give different results when applied to states in $\mathcal{H}$ since it is not necessarily the case that the spatial boundary operator: $\int d^3x \; \partial_i B^{i\mu}$ vanishes exactly. The only way to determine this definitively is to apply Theorem 1.

2.8 Response to Chapter 2

Following the publication of Ref. [1], on which Chap. 2 is based, the work has been discussed several times in the literature. Generally, this discussion has been performed in the context of whether or not the angular momenta operator has a physically meaningful decomposition. In Ref. [107] it is argued that the various ambiguities that arise when attempting to decompose nucleon spin, can be circumvented by working in a specific frame of reference. Nevertheless, the author concedes that in light of the analysis performed in [1], the appearance of spatial boundary terms can potentially cause problems. In Ref. [108] the ambiguities in the decomposition of nucleon spin are outlined, and a topological procedure is suggested in order to address these inconsistencies. The motivation for this approach comes mainly from the recognition that spatial boundary terms are not guaranteed to vanish, which is in part attributed to the analysis in [1]. Another notable discussion in the literature is Ref. [109]. Here the author instead raises the similar issue of the decomposition of the angular momentum of the photon, and proposes that potential ambiguities can be resolved by using the results of laser optics experiments. It is pointed out that the important issue of whether or not spatial boundary operators vanish has rarely been addressed in the literature, and that the analysis in [1] is one of the first attempts to solve this problem.

Overall, the relevance of this issues raised in Ref. [1] appear to have been recognised in the literature, and this has led to renewed discussion about whether or not the decomposition of nucleon spin is physically meaningful.

Chapter 3

Non-manifest symmetries in quantum field theory

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3.1 Abstract

Non-manifest symmetries are an important feature of quantum field theories, and yet their characteristics are not fully understood. In particular, the construction of the charge operators associated with these symmetries is ambiguous. In this paper we adopt a rigorous axiomatic approach in order to address this issue. It turns out that charge operators of non-manifest symmetries are not unique, and that although this does not affect their property as generators of the corresponding symmetry transformations, additional physical input is required in order to determine how they act on states. Applying these results to the examples of spacetime translation and Lorentz symmetry, it follows that the assumption that the vacuum is the unique translationally invariant state, is sufficient to uniquely define the charges associated with these symmetries. In the case of supersymmetry though there exists no such physical requirement, which means that the supersymmetric charge is not uniquely defined, and this therefore introduces a potential non-perturbative obstacle to the consistency of supersymmetric QFTs.

3.2 Introduction

Non-manifest symmetry is an important feature of quantum field theory (QFT), and yet the quantisation of these types of symmetries is still not fully understood. In particular, the question of which features of classical non-manifest symmetries survive quantisation remains unresolved. Given a classical field theory with fields $\{\varphi_a\}$ and Lagrangian density $\mathcal{L}$, a non-manifest symmetry is a symmetry for which $\delta\mathcal{L} = \partial_\mu \mathcal{B}^\mu$. The corresponding Noether current[1] has the form:

$$j^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_a)}\delta\varphi_a - \mathcal{B}^\mu \tag{3.1}$$

and its conservation $\partial_\mu j^\mu = 0$ follows from the Euler-Lagrange equations. Manifest symmetries are defined by the fact that $\mathcal{B}^\mu \equiv 0$, and so the current is canonically

[1] The Noether current may also have additional indices other than μ, but here we will use j^μ for simplicity.

determined [110]. But for non-manifest symmetries $\mathcal{B}^\mu$ is not defined to vanish, which means that there is the freedom to redefine $\mathcal{B}^\mu$ by performing the following *improvement* transformation[2]:

$$\mathcal{B}^\mu \longrightarrow \mathcal{B}^\mu + \partial_\nu \widetilde{\mathcal{B}}^{[\mu\nu]} \tag{3.2}$$

without changing $\delta\mathcal{L}$ or affecting the conservation of the current. However, because the current j^μ *is* modified, this freedom implies an ambiguity in the definition of j^μ [110]. Since the charges associated with these currents are defined by $Q = \int d^3x\, j^0(x)$, improvement terms in the current become spatial boundary terms $\int d^3x\, \partial_i \widetilde{\mathcal{B}}^{[0i]}$ in the charges. So if two currents j^μ and $\tilde{j}^\mu$ differ by an improvement term, it follows from Stokes' theorem that the corresponding charges Q and $\widetilde{Q}$ may be equal if the fields satisfy certain boundary conditions, such as the requirement to vanish at spatial infinity.

A significant difference between classical and quantum field theories is that quantised fields are operator-valued distributions, and not functions. An important consequence of this is that quantised fields are not point-wise defined [49]. The physical motivation for this feature is that because operators inherently imply a measurement, if a field $\varphi(x)$ *were* a well-defined operator then this would represent the performance of a measurement at a single spacetime point x. However, quantum mechanically this is not possible since this would require an infinite amount of energy [50]. Instead, one can perform a measurement over a spacetime region $\mathcal{U}$ and model this with the operator $\varphi(f) := \int d^4x\ \varphi(x)f(x)$, which consists of a distribution φ smeared with some test function f with support in $\mathcal{U}$. Quantised fields being operator-valued distributions is one of a series of axioms which are employed in axiomatic approaches to QFT. Although different axiomatic schemes have been proposed, these schemes generally consist of a common core set of axioms including, for example, local (anti-)commutativity and the uniqueness of the vacuum[3]. The requirement that these axioms are compatible with the definition of a quantised field is also another strong motivation for why these fields are distributions as opposed to functions[4]. Because of the distributional behaviour of

[2] $\partial_\nu \widetilde{\mathcal{B}}^{[\mu\nu]}$ is referred to as an *improvement term* [94], and $[\mu\nu]$ indicates that the indices μ and ν are anti-symmetric.

[3] See e.g. [49–51] for a more in-depth discussion.

[4] Assuming fields $\varphi(x)$ are operator-valued functions, and combining this with certain standard QFT axioms, implies $\exists c \in \mathbb{C}$ such that: $\varphi(x)|0\rangle = c|0\rangle\ \forall x$, and hence the fields cannot be non-trivial [60].

quantised fields, the arguments used to determine the characteristics of classical non-manifest symmetries are generally no longer valid for QFTs. In particular, since the spatial boundary terms $\int d^3x\, \partial_i \widetilde{\mathcal{B}}^{[0i]}$ are operators in the quantised theory, and imposing boundary conditions on quantised fields is ill-defined [1], the classical reasoning used to justify when these terms vanish does not apply. Nevertheless, these arguments are still often cited to explain the vanishing of these terms in QFT [42, 44, 95].

The remainder of this paper is structured as follows: in Sec. 3.3 we analyse the quantisation and general characteristics of non-manifest symmetries in QFTs; in Sec. 3.4 we apply these findings to specific examples of these symmetries; and finally in Sec. 3.5 we summarise our results.

3.3 Quantum non-manifest symmetries

3.3.1 Quantisation

As outlined in Sec. 3.2, spatial boundary operators are an important feature of quantum non-manifest symmetries. In classical field theories, these spatial boundary terms have the form $B = \int d^3x\ \partial_i B^i(x)$, where $B^i(x)$ is some field. However, since *quantised* fields are distributions, the quantum analogue of B must involve a smearing with test functions in order to yield a well-defined operator. Moreover, it is necessary that this smearing is performed both in space *and* time, since $\partial_i B^i(x)$ is in general not defined at sharp times [47]. The spatial boundary operator B can thus be written: $B = \int d^4x\ f(x)\partial_i B^i(x) = \partial_i B^i(f)$, where f is some test function on $\mathbb{R}^{1,3}$. As discussed in Sec. 3.2, the operator $B = \partial_i B^i(f)$ represents the performance of a measurement on the spacetime region $\mathrm{supp}(f) \subset \mathbb{R}^{1,3}$. Therefore, in order to ensure that B agrees with the classically-motivated form for B, and is defined on the whole of space, one can choose without loss of generality [1] that $f(x) := \alpha(x_0) f_R(\mathbf{x})$, where $\alpha \in \mathcal{D}(\mathbb{R})$ ($\mathrm{supp}\,(\alpha) \subset [-\delta, \delta]$, $\delta > 0$) and $f_R \in \mathcal{D}(\mathbb{R}^3)$ have the following properties:

$$\int dx_0\ \alpha(x_0) = 1, \qquad f_R(\mathbf{x}) = \begin{cases} 1, & |\mathbf{x}| < R \\ 0, & |\mathbf{x}| > R(1+\varepsilon) \end{cases} \tag{3.3}$$

with $\varepsilon > 0$. Hence the spatial boundary operator B has the explicit form:

$$B = \lim_{R\to\infty} \int d^4x \ \alpha(x_0) f_R(\mathbf{x}) \, \partial_i B^i(x) \tag{3.4}$$

As well as spatial boundary operators, this same class of test functions can also be used to rigorously define the quantum variation δF of a (smeared) field operator F under a symmetry transformation. Given that the symmetry gives rise to the conserved Noether current j^μ, δF is defined as follows [79, 98, 99]:

$$\delta F = i\,[Q, F]_\pm := \lim_{R\to\infty} i\,[Q_R, F]_\pm = \lim_{R\to\infty} i \left[j^0(\alpha f_R), F\right]_\pm \tag{3.5}$$

where Q_R is a localised expression for the charge generator Q of the symmetry, and $[\cdot,\cdot]_\pm$ is either an anti-commutator or commutator depending on the spin of Q and F.

It turns out that the definitions for both B and δF are not completely sufficient to ensure that these operators are always well-defined. One also requires that the algebra of fields $\mathcal{F}$ in the theory is *local*, which means that for any fields $\phi, \psi \in \mathcal{F}$, one has that $[\phi(f), \psi(g)]_\pm = 0$ when the supports of the test functions f and g are space-like separated[5]. However, the locality of $\mathcal{F}$ is not guaranteed for all classes of QFTs. In particular, for gauge theories it transpires that the gauge symmetry of the theory implies a strengthened form of the Noether current conservation condition, and this leads to the possibility of non-local fields [47]. A prominent example of this is quantum electrodynamics (QED) in the Coulomb gauge, where all the *charged* fields are non-local [75]. Nevertheless, it turns out the locality of the field algebra can be preserved, and this can be achieved by adopting a so-called *local quantisation* [47]. In local quantisations, additional degrees of freedom are introduced into the theory, resulting in an extension of the space of states $\mathcal{V}$. However, an important consequence of this extension is that the inner product in $\mathcal{V}$ is no longer positive definite. So the locality of $\mathcal{F}$ is preserved at the expense of violating the positivity of the inner product in $\mathcal{V}$. Since negative norm states are unphysical, one must therefore introduce a condition in order to determine the physical states $\mathcal{V}_{\text{phys}} \subset \mathcal{V}$. For Yang-Mills theories, *BRST quantisation* is an important example of a local quantisation. In this case ghost and gauge-fixing degrees of freedom are added to the theory in order to break the gauge invariance, and preserve the locality of $\mathcal{F}$. Although the gauge-fixed theory is no longer gauge invariant,

[5] This property is called local (anti-)commutativity.

it remains invariant under a residual *BRST* symmetry, with a corresponding conserved charge Q_B. Physical states are specified by the *subsidiary* condition: $Q_B\mathcal{V}_{\text{phys}} = 0$, and the corresponding Hilbert space is defined by $\mathcal{H} := \overline{\mathcal{V}_{\text{phys}}/\mathcal{V}_0}$, where $\mathcal{V}_0 \subset \mathcal{V}_{\text{phys}}$ contains the zero norm states[6].

Determining the conditions under which spatial boundary operators vanish is central to understanding the differences between classical and quantum non-manifest symmetries. This issue was first investigated for locally quantised QFTs in [1], where spatial boundary operators B were rigorously defined as in Eq. (3.4). It was established that if B annihilates the vacuum state, then this is both necessary and sufficient to ensure that $B = 0$, and hence one has the following theorem:

Theorem 2. $\int d^3x\ \partial_i B^i$ *vanishes in* $\mathcal{V} \iff \int d^3x\ \partial_i B^i|0\rangle = 0$

where $\int d^3x\ \partial_i B^i$ implicitly involves the smearing in Eq. (3.4). It should be noted that Theorem 2 differs slightly to the theorem derived in [1] in that it involves the state space $\mathcal{V}$, as opposed to $\mathcal{H}$. This subtle modification is necessary in order to ensure that the theorem is applicable to arbitrary locally quantised theories[7]. As already discussed in Sec. 3.2, given a classical non-manifest symmetry with canonical Noether current j^μ, one can modify j^μ by adding an improvement term $\partial_\nu\widetilde{\mathcal{B}}^{[\mu\nu]}$ without affecting its overall conservation. The corresponding charges Q and $\widetilde{Q}$ associated with j^μ and $\tilde{j}^\mu = j^\mu + \partial_\nu\widetilde{\mathcal{B}}^{[\mu\nu]}$ will therefore differ by a spatial boundary term, the vanishing of which will depend on the boundary conditions of the (classical) fields. In light of Theorem 2, it follows that spatial boundary *operators* are similarly not guaranteed to vanish, and this immediately implies the corollary:

Corollary 1. *The charge generator of a quantum non-manifest symmetry is a priori non-unique*

Corollary 1 runs contrary to the expectation of much of the established literature [42, 44, 94, 95], and has to our knowledge not been discussed before. This is in part because it is often incorrectly concluded that spatial boundary *operators* can be assumed to

[6]The bar implies that $\mathcal{H}$ also includes certain limit states [51].

[7]The requirement for this modification arises because the Reeh-Schlieder theorem, which is central to the proof of Theorem 2, holds in $\mathcal{V}$ but may no longer hold in $\mathcal{H}$, as discussed in [51].

vanish by imposing suitable *classical* boundary conditions. The non-uniqueness of a charge operator Q immediately implies that its action on states is ambiguous, since one can in principle always add an improvement term to the current such that the transformed charge $\widetilde{Q}$ is different to Q. This therefore provides a non-perturbative obstacle to the consistency of QFTs that are invariant under a non-manifest symmetry.

Before discussing the consequences of Corollary 1 for specific examples of quantum non-manifest symmetries, we will first explore the effect that the ambiguity in the charge has on the generation of the transformations associated with these symmetries. By using the definition of the quantum variation δF (Eq. (3.5)), one has the following theorem:

Theorem 3. *If* $\widetilde{Q} = Q + \int d^3x\ \partial_i B^i$*, where* Q *is a charge operator, then*

$$\widetilde{\delta} F := i[\widetilde{Q}, F]_\pm = i[Q, F]_\pm = \delta F$$

for all operators F *constructed from (local) fields smeared with some test function*

Proof. Let $|\Psi\rangle$ and $|\Phi\rangle$ be any arbitrary states, then

$$\begin{aligned}
\langle\Psi| \left([\widetilde{Q}, F]_\pm - [Q, F]_\pm\right)|\Phi\rangle &= \langle\Psi| \int d^3x \left[\partial_i B^i, F\right]_\pm |\Phi\rangle \\
&= \langle\Psi| \lim_{R\to\infty} \int d^4x\ \alpha(x_0) f_R(\mathbf{x}) \left[\partial_i B^i(x), F\right]_\pm |\Phi\rangle \\
&= -\langle\Psi| \lim_{R\to\infty} \int d^4x\ \alpha(x_0) \left(\partial_i f_R(\mathbf{x})\right) \left[B^i(x), F\right]_\pm |\Phi\rangle \\
&= -\langle\Psi| \lim_{R\to\infty} \left[B^i(\alpha\partial_i f_R), F\right]_\pm |\Phi\rangle = 0
\end{aligned}$$

where the vanishing in the last equality follows because the support of $\alpha\partial_i f_R$ and the test function in the smearing of F will become space-like separated in the limit $R \to \infty$, and both B^i and F satisfy local (anti-)commutativity. □

Theorem 3 implies that despite the ambiguity in the definition of the generators of quantum non-manifest symmetries, different charge operators are guaranteed to generate *the same* symmetry transformation. This is in contrast to the classical case, where invariance of the symmetry transformation[8] requires that the boundary conditions of the fields must be such that *all* spatial boundary terms are exactly vanishing.

Although Theorem 3 guarantees that different expressions for the charges of quantum non-manifest symmetries will generate the same transformation, Corollary 1, as outlined previously, implies that the action of charges on states themselves is potentially ambiguous. However, as a consequence of Theorem 2, one has the corollary:

Corollary 2. *If* $\widetilde{Q} = Q + \int d^3x\ \partial_i B^i$ *for charge operators* $\widetilde{Q}$ *and* Q*, then*

$$\widetilde{Q}|0\rangle = Q|0\rangle \quad \Longleftrightarrow \quad \widetilde{Q} = Q$$

Corollary 2 follows immediately from the fact that $\int d^3x\ \partial_i B^i$ vanishes if and only if it annihilates the vacuum state. Therefore, if any two charges that are related by an improvement transformation act in the same manner on the vacuum state, this is both necessary and sufficient to imply that these charges are equal. In other words, knowledge of how the charge operators of non-manifest symmetries act on the vacuum is sufficient to uniquely define them. This means that in contrast to manifest symmetries, where the conserved current and hence the charge Q are canonically determined (i.e. $\mathcal{B}^\mu \equiv 0$ in Eq. (3.1)), quantum non-manifest symmetries require additional physical input in order to specify Q.

3.3.2 Spontaneous symmetry breaking

An important feature of any QFT is the phenomenon of spontaneous symmetry breaking (SSB). In general, the criterion for a quantum symmetry to be spontaneously broken can be characterised by the theorem [76]:

Theorem 4. *A symmetry is spontaneously broken* $\quad \Longleftrightarrow \quad \exists\, \varphi \in \mathcal{F}$ *such that* $\langle \delta\varphi \rangle \neq 0$

[8]For classical field theories, Poisson brackets are instead used to define the symmetry transformation δF.

where $\mathcal{F}$ is the (local) space of fields in the theory, δ is the symmetry variation defined in Eq. (3.5), and $\langle \cdot \rangle$ is the vacuum expectation value. In light of Corollary 1, it is important to establish whether there is a subsequent ambiguity in determining whether a non-manifest symmetry is spontaneously broken or not. As a consequence of Theorems 3 and 4, one has the following corollary:

Corollary 3. *The criterion for a non-manifest symmetry to be spontaneously broken is independent of the choice of charge*

This means that although the charges Q of non-manifest symmetries are in general not unique, since it is always possible to perform an improvement transformation $Q \to \widetilde{Q}$, one can equally use any of these charges to establish whether SSB occurs (via Theorem 4) without ambiguity.

Often SSB is characterised by the action of the charge Q on the vacuum state, and in particular that SSB occurs if and only if $Q|0\rangle \neq 0$ [19, 20]. However, the problem with this condition is that unlike Theorem 4, the action of Q on the vacuum state is *not* invariant under improvement transformations $Q \to \widetilde{Q}$, and is therefore ambiguous for non-manifest symmetries. In fact, due to Corollary 2, knowledge of $Q|0\rangle$ is required in order to uniquely define Q in the first place. Therefore, if it were true that SSB could be solely characterised by $Q|0\rangle$, then this would mean that the physical input required to define Q would automatically *also* determine whether the symmetry is spontaneously broken or not. But this cannot be the case, because this would imply that every non-manifest symmetry could only either always be broken or always unbroken, but not both.

3.4 Examples of quantum non-manifest symmetries

As outlined in Sec. 3.3, quantum non-manifest symmetries have many interesting and subtle features. In this section we will discuss these features in the context of some prominent examples of these symmetries.

3.4.1 Translational invariance

The invariance of a QFT under spacetime translations is an important example of a quantum non-manifest symmetry. In this case, the conserved current is the energy-momentum tensor $T^{\mu\nu}$ and the corresponding charge is the energy-momentum operator P^{μ}. By applying the results of Sec. 3.3, and in particular Theorem 2 and Corollary 1, it follows that $T^{\mu\nu}$, and hence P^{μ}, are ambiguously defined. Nevertheless, it is frequently cited in the literature [42, 94, 95] that one can always add an improvement term to $T^{\mu\nu}$ without modifying the corresponding charge. A prominent example of this is the symmetric Belinfante energy-momentum tensor $T_{B}^{\mu\nu}$ and the canonical current $T_{c}^{\mu\nu}$, which are related (by an improvement term) as follows [93]:

$$T_{B}^{\mu\nu} = T_{c}^{\mu\nu} + \partial_{\rho}G^{[\mu\rho]\nu}$$

Now although Theorem 3 implies that the corresponding charges P_{B}^{μ} and P_{c}^{μ} are both generators of translations, it is not necessarily the case that these operators act in the same manner on states[9]. This in fact highlights a deeper problem – *how does one determine which energy-momentum operator is correct?* It is clear that in order to answer this question one requires additional physical information[10]. In QFTs, the energy-momentum operator P^{μ} plays a special role in characterising the vacuum state $|0\rangle$. In particular, axiomatic formulations of QFT assume $|0\rangle$ to be the unique translationally invariant state [49–51], which means it satisfies the condition: $P^{\mu}|0\rangle = 0$. Since Corollary 2 implies that P^{μ} is uniquely defined by its action on $|0\rangle$, this condition provides a solution to the problem of which energy-momentum operator is physically relevant. In other words, if one can demonstrate that a certain expression for P^{μ} (e.g. P_{B}^{μ} or P_{c}^{μ}) annihilates the vacuum, then this is sufficient to prove that this is the only charge that satisfies this property, and must therefore be *the* physical energy-momentum operator.

[9]This potential difference between P_{B}^{μ} and P_{c}^{μ} has been largely ignored in the literature, but has been emphasised before in [89].

[10]It is sometimes concluded that the Belinfante generator is more physically motivated because $T^{\mu\nu}$ is symmetric when defined as the variational derivative of the action with respect to the metric in General Relativity. However, as pointed out in [89], $T^{\mu\nu}$ need not be symmetric if one loosens the requirement that $g^{\mu\nu}$ is symmetric and covariantly constant ($\nabla_{\sigma}g^{\mu\nu} = 0$), as is the case in Einstein-Cartan theory.

3.4.2 Lorentz invariance

Invariance under Lorentz transformations is another example of a non-manifest symmetry. The conserved current is $M^{\mu\nu\lambda}$, and the corresponding charge is $M^{\mu\nu}$. Just like with the energy-momentum tensor, one has both Belinfante $M_B^{\mu\nu\lambda} = x^\nu T_B^{\mu\lambda} - x^\lambda T_B^{\mu\nu}$ and canonical $M_c^{\mu\nu\lambda}$ currents which are both conserved, and differ by an improvement term. Similarly, it follows from the conclusions in Sec. 3.3 that the charges $M_B^{\mu\nu}$ and $M_c^{\mu\nu}$ are both generators of Lorentz transformations, but are not necessarily the same operator. This again raises the same problem of how to establish which charge is physically relevant. As discussed in Sec. 3.4.1, axiomatic formulations of QFT assume that the vacuum state $|0\rangle$ is the unique translationally invariant state. It transpires that this assumption implies that $|0\rangle$ is *also* invariant under Lorentz transformations [47], and hence $M^{\mu\nu}|0\rangle = 0$. Due to Corollary 2, this physical condition therefore provides a way in which $M^{\mu\nu}$ can be uniquely determined. It should be noted that although the conditions $P^\mu|0\rangle = 0$ and $M^{\mu\nu}|0\rangle = 0$ appear relatively simple, their verification is not necessarily straight-forward, especially in QFTs such as quantum chromodynamics (QCD) where the vacuum state has a non-trivial structure [37]. Nevertheless, in principle these conditions could be verified using a non-perturbative approach such as lattice QFT.

Much of the discussion in the literature regarding the current $M^{\mu\nu\lambda}$ centres around the construction of angular momentum operators $J^i = \frac{1}{2}\epsilon^{ijk}\int d^3x\, M^{0jk}$. In particular, an open problem in QCD which has received both significant theoretical and experimental focus, is the question of whether the angular momentum operator J_{QCD} has a meaningful decomposition into separate quark and gluon contributions [81, 85, 88, 89]. There are many different proposed decompositions of J_{QCD}, but they all have in common the fact that they are constructed by adding improvement terms to the canonical $M_c^{\mu\nu\lambda}$ or Belinfante $M_B^{\mu\nu\lambda}$ Lorentz currents. Although it remains uncertain which (if any) of these decompositions is physically meaningful [1, 89], this is directly related to issue of whether certain spatial boundary operators vanish or not. Ultimately, if the physical Lorentz charge $M^{\mu\nu}$ (where $M^{\mu\nu}|0\rangle = 0$) could be determined, this would be significant step in answering this question.

3.4.3 Supersymmetry

Supersymmetry corresponds to an enlargement of the Poincaré group of spacetime symmetries, and is another prominent example of a non-manifest symmetry. Invariance under supersymmetric transformations implies a conserved current S^{μ}_{α}, which gives rise to a spinor-valued charge Q_{α}. An important feature of supersymmetric QFTs is that unlike the operators P^{μ} and $M^{\mu\nu}$ in non-supersymmetric theories, there is no equivalent physical requirement as to how Q_{α} (or $Q^{\dagger}_{\alpha}$) should act on the vacuum state. If one were to similarly assume on physical grounds that $Q_{\alpha}|0\rangle = 0$ (and $Q^{\dagger}_{\alpha}|0\rangle = 0$), then this would imply:

$$\langle \delta\varphi \rangle = 0, \quad \forall \varphi \in \mathcal{F}$$

and hence any physical supersymmetric QFT would have to have unbroken supersymmetry. The problem with this criterion is that unlike Poincaré symmetry, SSB plays a particularly important role in the characterisation of physically realistic supersymmetric theories. The reason for this is that the supersymmetry algebra implies that every known particle must have a corresponding supersymmetric partner, with equal mass [19, 20]. Since these additional particles have never been observed, it is concluded that supersymmetry must be spontaneously broken [19, 20], and so this rules out $Q_{\alpha}|0\rangle = 0$ as a general physical criterion. So if such a criterion did exist then it would necessarily have to imply that $Q_{\alpha}|0\rangle$ is a non-vanishing state. But since there is no clear physical principle as to what state $Q_{\alpha}|0\rangle$ should be, it follows from Corollaries 1 and 2 that:

Corollary 4. *The supersymmetric charge Q_{α} is non-unique*

Due to Theorem 3 and Corollary 3, the ambiguity in the definition of Q_{α} does not affect the generation of supersymmetric transformations, nor the determination of whether the supersymmetry is spontaneous broken or not. Nevertheless, because the structure of Q_{α} is not fixed, the action of Q_{α} on states is not uniquely defined. Ultimately, this means that the supersymmetric space of states cannot be constructed in a consistent manner, and this therefore provides a non-perturbative obstacle to the consistency of supersymmetric QFTs.

3.5 Conclusions

Non-manifest symmetries play an important role in QFT, and yet the quantisation of these symmetries is still not fully understood. Although it well known that the ambiguity in the definition of the conserved currents associated with these symmetries provides the freedom to define different charges, often classical arguments are incorrectly employed to justify that these charge operators are physically equivalent. The central issue in this regard is to determine the conditions under which spatial boundary operators vanish. It turns out that for locally quantised theories, there in fact exists both a necessary and sufficient condition for when this class of operators vanishes. By applying this condition it follows that the charge operators of non-manifest symmetries are non-unique, but different expressions for the charge operator still generate the same symmetry transformations. In the context of SSB, these results ensure that in spite of the non-uniqueness of the charge, the criterion for SSB is not affected by this ambiguity. Nevertheless, the charge non-uniqueness is still potentially problematic because it remains unclear as to how the charge operator acts on states. A prominent example of this is the definition of the energy-momentum P^{μ} and Lorentz charges $M^{\mu\nu}$ associated with the non-manifest symmetries of spacetime translation and Lorentz invariance. In each case, both canonical and Belinfante charges can be defined, but it is unclear which of these operators (if either) is more physically relevant. A possible solution to this problem is to use the physical assumption that the vacuum is the unique translationally invariant state, because it follows that a knowledge of how these operators act on the vacuum is enough to uniquely define them. However, in the case of supersymmetry, there is no such physical requirement as to how the supersymmetric charge Q_{α} should act on the vacuum. So by contrast to P^{μ} and $M^{\mu\nu}$, Q_{α} is *not* uniquely defined, and this therefore introduces a potential non-perturbative obstacle to the consistency of supersymmetric QFTs.

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3.6 Appendix

3.6.1 The spaces $\mathcal{H}$ and $\mathcal{V}$

In Sec. 3.3.1 it was noted that Theorem 2 differs slightly in form to Theorem 1 in Chap. 2, since it involves the indefinite inner product state space $\mathcal{V}$, as opposed to $\mathcal{H}$. Here I will explain in more detail why this modification is necessary. In the case of locally quantised gauge theories with charges Q^a, it turns out that if $|\Psi\rangle$ is a *localised* physical state (in $\mathcal{H}$) constructed using operators in $\mathcal{F}(\mathcal{O})$ where $\mathcal{O} \subset \mathbb{R}^{1,3}$ is some bounded spacetime region (see Sec. 1.2.3), it follows that $Q^a|\Psi\rangle = 0$ [51]. In the case of QED this implies that every localised physical state is neutral, and in QCD that these states are colourless[11]. An important question is whether this condition *also* holds for *non-localised* physical states. For QCD this would certainly make physical sense because it would prevent the existence of any coloured physical state (local or non-local), and thus imply confinement. However, if this were true for QED then it would inevitably prohibit the existence of charged physical states such as the electron.

This issue is made subtle by the Reeh-Schlieder Theorem (see Sec. 1.2.3), which for locally quantised QFTs implies that *any state* can be approximated as a limit of localised states in $\mathcal{V}$. In particular, this means that given some non-localised state $|\Phi\rangle$, this state can *always* be approximated to arbitrary precision using localised states $\{|\Phi_n\rangle\}$ in $\mathcal{V}$. The important point is whether this approximation can be performed using localised limiting states contained entirely within $\mathcal{H}$ or not. If it can, then it immediately follows that $Q^a|\Phi\rangle = 0$ (since $Q^a|\Phi_n\rangle = 0, \forall n$), and hence *all* physical states must be chargeless. If it cannot, then charged physical states are permitted. By assuming that the Reeh-Schlieder Theorem holds in $\mathcal{H}$ it follows that all limiting states $\{|\Phi_n\rangle\}$ are also in $\mathcal{H}$, and hence the former condition must be satisfied. However, since it is unknown for an arbitrary (locally quantised) theory as to whether charged physical states can exist or not, one cannot assume that the Reeh-Schlieder Theorem always holds in $\mathcal{H}$. This is the reason why one must instead use the more general state space $\mathcal{V}$ in Theorem 2. In the proof of Theorem 1 though, it *is* implicitly assumed that the Reeh-Schlieder Theorem holds in $\mathcal{H}$. However, since Theorem 1 is discussed solely in the context of

[11] This assumes that these symmetries are not spontaneously broken.

QCD in Chap 2, it is likely that the Reeh-Schlieder Theorem does in $\mathcal{H}$ in this case, and therefore no generality is lost.

3.6.2 Non-manifest symmetry structure

In Sec. 3.4, the general results for the charges of non-manifest symmetries derived in Sec. 3.3 are applied to some prominent non-manifest symmetry examples including: translational invariance, Lorentz invariance, and supersymmetry. Here the classical non-manifest structure of these symmetries will be briefly described. For simplicity, consider the case of a scalar field theory with fields $\{\phi_a(x)\}$. In the case of (infinitesimal) translational invariance $x^\nu \to x^\nu - \epsilon^\nu$, the fields transform as: $\phi_a(x) \to \phi_a(x) + \epsilon^\nu \partial_\nu \phi_a(x)$. Since the Lagrangian density $\mathcal{L}(x)$ is itself a Lorentz scalar, it similarly transforms as: $\mathcal{L}(x) \to \mathcal{L}(x) + \epsilon^\nu \partial_\nu \mathcal{L}(x)$, and hence: $\delta\mathcal{L} = \partial_\mu(\delta^\mu_\nu \epsilon^\nu \mathcal{L})$. From the discussion in Sec. 3.2, this directly confirms that spacetime translational invariance is a non-manifest symmetry, and in this case:

$$\mathcal{B}^\mu = \delta^\mu_\nu \epsilon^\nu \mathcal{L}$$

For (infinitesimal) Lorentz invariance, the components of the Lorentz transformation Λ can be decomposed as follows: $\Lambda^\mu_\nu = \delta^\mu_\nu + \omega^\mu_\nu$, where $\omega^{\mu\nu}$ is anti-symmetric. The field $\phi_a(x)$ transformation as: $\phi_a(x) \to \phi_a(x) - \omega^\mu_\nu x^\nu \partial_\nu \phi_a(x)$, and due to the anti-symmetry of $\omega^{\mu\nu}$ it follows that: $\delta\mathcal{L} = \partial_\mu(-\omega^\mu_\nu x^\nu \mathcal{L})$, and hence:

$$\mathcal{B}^\mu = -\omega^\mu_\nu x^\nu \mathcal{L}$$

which implies that Lorentz invariance is also a non-manifest symmetry.

One of the simplest examples of a supersymmetric theory is $\mathcal{N} = 1$ supersymmetric Yang-Mills. This theory is a minimal supersymmetric gauge theory [19], and the Lagrangian density has the form: $\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{\mu\nu a} - \frac{1}{2} \overline{\Psi}^a \not{D} \Psi^a$, where the fermion fields Ψ^a are Lie algebra-valued, and $F^a_{\mu\nu}$ is the field strength tensor of the Yang-Mills field field A^a_μ. In this theory the supersymmetry transformations of the fields are defined by:

$$\delta A^a_\mu = \bar{\epsilon}\gamma_\mu \Psi^a \qquad \delta\Psi^a = -\tfrac{1}{4}\epsilon \left[\gamma^\alpha, \gamma^\beta\right] F^a_{\alpha\beta}$$

where ϵ and $\bar{\epsilon}$ are constant (infinitesimal) Majorana spinors. Under these transformations it follows that: $\delta\mathcal{L} = \partial_\mu \left(-\frac{1}{4}\bar{\epsilon}\gamma^\mu\sigma^{\alpha\beta}F^a_{\alpha\beta}\Psi^a\right)$ and thus:

$$\mathcal{B}^\mu = -\frac{1}{4}\bar{\epsilon}\gamma^\mu\sigma^{\alpha\beta}F^a_{\alpha\beta}\Psi^a$$

In fact, as discussed in [20], the non-vanishing of $\mathcal{B}^\mu$ is actually essential to guarantee the consistency of *any* supersymmetric theory.

Overview of Chapters 4 and 5

As outlined in the overview to Chaps. 2 and 3, this thesis involves a series of investigations into different problems in particle physics, with the aim of using an axiomatic QFT approach in order to achieve a better understanding. In these chapters, critical issues surrounding the spin structure of hadrons [1] and the quantisation of non-manifest symmetries [3] were explored. As is the case for Chaps. 2 and 3, Chaps. 4 and 5 are also comprised of publications ([2] and [4] respectively), and are therefore deliberately self-contained and concise. Since both of these chapters explore similar topics and involve some of the same structural relations, the salient technical features will be outlined again here. Moreover, in order to further motivate the relevance of these works, the context of the work with regards to the literature will be described, together with the main themes involved.

In Chap. 1, the general mathematical structure of QFTs is described, as well as some of the more important non-perturbative consequences they imply. A consequence of particular importance is the Reconstruction Theorem [49], which roughly speaking implies that a QFT can be fully understood if one knows the behaviour of all the Wightman functions. This remarkable result justifies why the understanding of the structure of these objects is of central importance in QFT. A significant milestone in the study of Wightman functions, and in particular correlators (two-point functions), was the discovery of the *spectral representation* [111–114]. In general, this is a (momentum space) integral representation of a correlator which consists of a convolution between free field correlators and spectral densities $\rho(s)$. This representation arises because the Fourier transform of a correlator $\widehat{T}_{(1,2)}(p) = \mathcal{F}\left[\langle 0|\phi_1(x)\phi_2(y)|0\rangle\right]$ is a Lorentz covariant tempered distributions $\mathcal{S}'(\mathbb{R}^{1,3})$ with support in the closed forward light cone $\overline{V}^+$, as discussed in Chap. 1. In the special case where $\widehat{T}_{(1,2)}(p)$ is specifically Lorentz invariant, the spectral representation has the following form [56]:

$$\widehat{T}_{(1,2)}(p) = P(\partial^2)\delta(p) + \int_0^\infty ds\, \theta(p^0)\delta(p^2 - s)\rho(s) \tag{3.6}$$

where $P(\partial^2)$ is some polynomial in the d'Alembert operator $\partial^2 = g_{\mu\nu}\frac{\partial}{\partial p_\mu}\frac{\partial}{\partial p_\nu}$, and $\rho(s) \in \mathcal{S}'(\bar{\mathbb{R}}_+)$. This representation can then be (inverse) Fourier transformed back into position space, and the resulting expression is the familiar *Källén-Lehmann representation* [111, 112][12]

$$\langle 0|\phi_1(x)\phi_2(y)|0\rangle = \int_0^\infty ds\, \rho(s)\, i\Delta^+(x-y;s) \tag{3.7}$$

where: $i\Delta^+(x-y;s) = \mathcal{F}^{-1}\left[\theta(p^0)\delta(p^2-s)\right]$. One of the nice features of this representation is that its existence is guaranteed by the QFT axioms, and this implies that it must hold both in perturbative and non-perturbative regimes.

In Chap. 4 the focus is on field propagators, which as opposed to correlators involve vacuum expectation values of *time-ordered* products of fields $\langle 0|T\{\phi_1(x)\phi_2(y)\}|0\rangle$. In the case of a scalar field theory, the Källén-Lehmann representation of the propagator has precisely the form of Eq. (3.7), where instead $i\Delta^+(x-y;s)$ is replaced with the free Feynman propagator $i\Delta_F(x-y;s)$ [95]. However, in the case of propagators such as the quark propagator, which is also considered in Chap. 4, one has a more general situation where $\widehat{T}_{(1,2)}(p)$ is Lorentz *covariant*, but not Lorentz invariant. Therefore, the structure of $\widehat{T}_{(1,2)}(p)$ is dependent upon how the fields ϕ_1 and ϕ_2 transform under Lorentz transformations. It turns out that $\widehat{T}_{(1,2)}(p)$ has the following decomposition: $\widehat{T}_{(1,2)}(p) = \sum_{\alpha=1}^{\mathscr{N}} Q_\alpha(p)\, \widehat{T}_{\alpha(1,2)}(p)$, where $\widehat{T}_{\alpha(1,2)}(p)$ are Lorentz *invariant* distributions, and $Q_\alpha(p)$ are Lorentz covariant polynomial functions of p which carry the Lorentz index structure of ϕ_1 and ϕ_2 [56]. In this case this means that only the components $\widehat{T}_{\alpha(1,2)}$ of $\widehat{T}_{(1,2)}$ actually satisfy Eq. (3.6). For the quark propagator $\langle 0|T\{\psi(x)\overline{\psi}(y)\}|0\rangle$, the corresponding Lorentz covariant polynomial functions are the spinor identity $\mathbb{I}$ and

[12] For QFTs with a positive-definite inner product $P(\partial^2)\delta(p)$ is at most some positive multiple of $\delta(p)$, and can be removed by rescaling the field [56]. However, for arbitrary indefinite inner product QFTs $P(\partial^2)\delta(p)$ can indeed play a role, but this will not be discussed further here.

$\gamma^\mu p_\mu = \not{p}$, and this implies that the propagator has the following spectral representation:

$$\langle 0|T\{\psi(x)\overline{\psi}(y)\}|0\rangle = \int_0^\infty ds\ \rho_V(s)\, iS_F(x-y;s) + i\Delta_F(x-y;s)\Big[\rho_S(s) - \sqrt{s}\,\rho_V(s)\Big] \tag{3.8}$$

where $iS_F(x-y;s)$ is the free fermionic Feynman propagator. In interacting QFTs, renormalisation of the fields is required in order to remove the divergences which arise as a result of the product of fields being ill defined at coincident space-time points. Nevertheless, one expects (renormalised) interacting QFTs like QCD to also obey some modified version of the Wightman axioms (see Sec. 1.2.4). This means that the correlators and propagators in these theories will therefore also possess spectral representations. However, the spectral densities ρ_α in this case must necessarily depend on how the fields are renormalised, and will therefore implicitly depend on the renormalisation scheme and renormalisation parameter μ [115]. Regardless of the theory, an important property of the spectral representation is that the structure of correlators or propagators is determined by the form of the corresponding spectral densities ρ_α. Determining the structure of spectral densities is therefore crucial to understanding the properties of *any* QFT, and this is why the analysis of spectral densities forms a key component of the investigations both in Chaps. 4 and 5.

Another important structural relation in QFT, which in particular plays a key role in Chap. 4, is the operator product expansion (OPE). The OPE was first proposed by Wilson [116] to describe the behaviour of products (or time-ordered products) of fields in the limit of coinciding space-time arguments. Given the (renormalised) fields $A(x)$ and $B(y)$, the OPE asserts that in the limit $x \to y$, the product $A(x)B(y)$ can be replaced by the sum $\sum_{i=1}^{n} \widetilde{C}_i(x-y)\widetilde{\mathcal{O}}_i(y)$ in any correlation function, where $\{\widetilde{\mathcal{O}}_i(y)\}_{i=1}^{n}$ is a finite set of fields, and $\widetilde{C}_i$ are (possibly singular) functions called the *Wilson coefficients*. A key feature of the OPE is that both the fields $\widetilde{\mathcal{O}}_i(y)$ and the Wilson coefficients $\widetilde{C}_i$ depend on the renormalisation parameter μ [117]. Conceptually, the OPE provides a factorisation of short and long distance degrees of freedom (above and below the scale $1/\mu$), which in the case of asymptotically free theories such as QCD, are partitioned between the Wilson coefficients and field operators $\widetilde{\mathcal{O}}_i$ respectively [118]. The coefficients $\widetilde{C}_i$ are computable using perturbation theory, and in particular are determined by the *renormalisation group equation* (RGE):

$$\mu \frac{d}{d\mu} \widetilde{C}_i = -\gamma_{ji} \widetilde{C}_j \tag{3.9}$$

The RGE arises due to the multiplicative renormalisation of the fields. In other words, the fact that renormalisation can be performed by rescaling the fields: $\varphi_0 = Z_\varphi \varphi_R$, where φ_0 is the bare (non-renormalised) field and Z_φ is some suitably chosen function of μ, implies that the correlators involving the renormalised fields φ_R, and hence the Wilson coefficients $\widetilde{C}_i$, must satisfy a differential equation in the parameter μ [117]. The behaviour of the solutions of Eq. (3.9) are controlled by the *anomalous dimensions* $\{\gamma_{ji}\}$, which characterise the fact that fields mix under renormalisation [117]. Once the form of the Wilson coefficients are established, the OPE provides a powerful tool with which one can analyse products of fields, and hence correlators.

In Chap. 4, a procedure is developed to extract novel information about the structure of correlation functions, and in particular spectral densities, by using both the spectral representation and the OPE. As detailed in Chap. 4, this procedure essentially involves performing a matching of the x-coefficients of the short distance expansion of the spectral representation of a propagator, with its corresponding OPE. It turns out that for each order of x considered in the expansions, one obtains a constraint on a specific moment of the spectral density. This procedure is in some sense similar to a successful technique which has already been used extensively in the study of hadronic physics – the Shifman-Vainstein-Zakharov (SVZ) approach [119]. The SVZ approach establishes sum rules, which are relations between hadronic parameters (decay constants f_h, hadronic masses m_h, and continuum thresholds s_0) and OPE parameters (quark masses and condensates). The SVZ procedure first involves defining a general ansatz for the *a priori* unknown spectral density ρ of the correlator, in terms of the parameters f_h, m_h and s_0. By then calculating the OPE of the correlator, a sum rule is formed by performing a Borel transformation of both the OPE and spectral representation [119–121]. The advantage of performing a Borel transformation is that the asymptotic OPE series is transformed into a convergent series depending on a free parameter M, the so-called *Borel parameter*. Moreover, the transformation exponentially suppresses the contributions to the spectral density from continuum states heavier than m_h. By relating OPE and hadronic parameters, the SVZ approach enables the determination of a wide variety of different observables. An important example is the pion decay constant f_π, which plays a key role in many low energy processes, including the strength of leptonic pion decays such as: $\pi^- \to e^- \bar{\nu}_e$ [122]. The SVZ sum rule for f_π has the following form [121]:

$$f_\pi^2 = M^2 \left[\frac{1}{4\pi^2} \left(1 - e^{-\frac{s_0^\pi}{M^2}} \right) \left(1 + \frac{\alpha_s}{\pi} \right) + \frac{1}{12M^4} \langle \frac{\alpha_s}{\pi} G_{\mu\nu}^2 \rangle + \frac{176\pi\alpha_s}{81M^6} \langle \bar{\psi}\psi \rangle^2 \right]$$

Therefore, once one has determined estimates for the quark and gluon condensates (e.g. using lattice QFT calculations), as well as the strong coupling α_s and the continuum threshold s_0^π, this relation allows one to directly calculate a theoretical prediction for f_π. Although the SVZ approach has certainly been successful, an advantage of the procedure developed in Chap. 4 is that constraints are imposed on the spectral density in a model independent manner, i.e. without assuming a parametrisation for ρ. Moreover, the procedure does not require a Borel transformation, and hence the introduction of the (*a priori* unknown) Borel parameter M, which is known to introduce one of the dominant uncertainties in the determination of hadronic parameters such as f_π [121]. In order to explicitly demonstrate the utility of this procedure, in the remainder of Chap. 4 the procedure is applied to the scalar propagator in ϕ^4-theory and the quark propagator in QCD, and its non-perturbative implications are outlined.

In Chap. 5, the asymptotic growth of correlation functions is explored, and in particular the so-called *cluster decomposition theorem*. This theorem describes how the strength of the correlations between field clusters depends on the distance between the clusters for large space-like distances. For QFTs that satisfy the Wightman axioms the correlation strength always *decreases* the further the clusters are separated [123], whereas for QFTs with a state space with an indefinite inner product, such as those described in Sec. 1.2.4, the correlation strength is permitted to *increase* under certain conditions [77]. This is particularly interesting in the context of QCD, since an increase in the correlation strength for correlators of clusters involving coloured fields implies that the strength of the correlations between the coloured degrees of freedom in these clusters increases at large distances. Therefore, the measurement of a state associated with one of the coloured fields cannot be performed independently of the other, which is a sufficient condition for confinement [40, 51]. In Chap. 5 a general criterion for the correlation strength of a cluster correlator to increase is derived. It turns out that this behaviour is related to the structure of the spectral densities $\rho(s)$ of any correlator involving coloured fields, such as the quark and gluon propagators. Although the exact non-perturbative structure of correlators such as these is unknown, methods such as lattice QCD and the Dyson-Schwinger equations (DSEs) provide an approximate way in which one can probe their behaviour, and thus test the confinement criterion derived in Chap. 5.

Lattice QFT consists of defining a QFT on a discretised spacetime lattice. In practical terms, this is achieved by using the (Euclidean) path integral formulation of QFT. The path integral is characterised by the generating functional:

$$Z[J] = \int d\mu \, e^{(J,\phi)} := \frac{1}{Z} \int \prod_x d\phi(x) \, e^{-S[\phi]+(J,\phi)} \tag{3.10}$$

where: $Z = \int \prod_x d\phi(x) \, e^{-S[\phi]}$, and $S[\phi]$ is the (classical) action of the theory [53]. The idea is that: $\langle 0|F[\phi]|0\rangle = \int d\mu \, F[\phi]$, which means that the vacuum expectation values of functionals of the fields F (e.g. n-point functions) are different moments of the field space measure[13] $d\mu$. By construction, the n-point functions of the theory are generated by taking functional derivatives of $Z[J]$ with respect to J, i.e. $\langle 0|\phi(x_1)\cdots\phi(x_n)|0\rangle = \frac{\delta^n Z[J]}{\delta J(x_1)\cdots\delta J(x_n)}\Big|_{J=0}$ (in a scalar field theory). If one can consistently construct the generating functional for a QFT, the n-point functions and thus the dynamics of the theory can be computed. For interacting theories this is a difficult problem, and boils down to defining a consistent measure $d\mu$. In lattice QFT the measure $d\mu$ is constructed on a spacetime lattice. This is achieved by discretising the fields $\phi(x)$ (often by imposing periodic boundary conditions) as well as the (Euclidean) action $S[\phi]$ and the field space measure $\prod_x d\phi(x)$. In doing so this introduces a cut-off in the momentum spectrum, and permits the calculation of non-perturbative quantities such as condensates[14]. Of course, since physical QFTs are defined in (continuous) spacetime, one must take the limit as the lattice spacing goes to zero (or cut-off goes to infinity). This is achieved by performing calculations on lattices with increasingly finer lattice spacings, and demonstrating that the results converge. The disadvantage with this approach though is that it is often computationally expensive, and there are always inherent uncertainties associated with using a finite (non-vanishing) lattice spacing [53, 54]. Moreover, the calculations in lattice QFT are always performed in Euclidean spacetime, since the path integral doesn't exist in Minkowski spacetime [55]. This means that one must eventually Wick rotate the results back to Minkowski space-

[13]See [55] for a rigorous definition of the measure $d\mu$.
[14]See [53–55] for a more in-depth discussion.

time. However, it is not guaranteed that this is always possible[15], and this remains one of the fundamental issues in lattice QFT. Nevertheless, lattice QFT has the potential to calculate non-perturbative quantities, including the propagators in QCD [124].

An alternative non-perturbative method is the Dyson-Schwinger equations (DSEs). Like lattice QFT, this approach also makes use of the path integral formulation. In particular, since the functional integral of a total derivative vanishes, it follows that the following differential equation must hold [125]:

$$\left[\frac{\delta S}{\delta\phi}\left(-\frac{\delta}{\delta J}\right)+J\right]Z[J]=0 \tag{3.11}$$

This is called the Dyson-Schwinger equation (for a scalar field). The interesting characteristic of this equation is that it leads to a coupled relation involving the exact (non-perturbative) propagator and the proper vertex (or effective action) $\Gamma[\phi]$, which is defined by: $Z[J]=e^{-\Gamma[\phi]+(J,\phi)}$. By using an ansatz for Γ this then enables one to solve the equation analytically for the propagator. However, in practice this is a difficult procedure, which often requires approximations to be made and the equations to be solved using some numerical procedure [125]. In the context of QCD, the DSEs are particularly interesting since they provide a powerful approach for determining the approximate structure of QCD propagators.

The preceding discussions demonstrate that both Lattice QFT and the DSEs are capable of providing an approximate determination of the non-perturbative structure of QCD propagators. This is of particular relevance in Chap. 5, where the quantities of interest are the so-called Schwinger functions: $C(t)=\int_0^\infty ds\,\rho(s)\frac{e^{-\sqrt{s}\,t}}{2\sqrt{s}}$ $(t\geq 0)$, which can be written in the form: $C(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dp_0\,e^{ip_0t}\Delta(p^2)|_{\mathbf{p}=0}$, where $\Delta(p^2)$ is one of the components of either the quark or gluon propagators. Therefore, by either performing a lattice calculation, or solving the DSEs in QCD, an approximation to $\Delta(p^2)$ can be determined, and this in turn enables the computation of $C(t)$ [126, 127]. It turns out that $C(t)$ has distinctive qualitative features, and these are important with regards to QCD confinement, as detailed in Chap. 5.

[15]See Sec. 1.2.3.

Chapter 4

Spectral density constraints in quantum field theory

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4.1 Abstract

Determining the structure of spectral densities is important for understanding the behaviour of any quantum field theory (QFT). However, the exact calculation of these quantities often requires a full non-perturbative description of the theory, which for physically realistic theories such as quantum chromodynamics (QCD) is currently unknown. Nevertheless, it is possible to infer indirect information about these quantities. In this paper we demonstrate an approach for constraining the form of spectral densities associated with QFT propagators, which involves matching the short distance expansion of the spectral representation with the operator product expansion (OPE) of the propagators. As an application of this procedure we analyse the scalar propagator in ϕ^4-theory and the quark propagator in QCD, and show that constraints are obtained on the spectral densities and the OPE condensates. In particular, it is demonstrated that the perturbative and non-perturbative contributions to the quark condensate in QCD can be decomposed, and that the non-perturbative contributions are related to the structure of the continuum component of the scalar spectral density.

4.2 Introduction

Spectral representations of matrix elements were first investigated by Källén [111], Lehmann [112], and then later by [113] and [114] among others. An important consequence of these investigations was the discovery of the *Källén-Lehmann representation* of the two-point function. For an arbitrary quantum field Ψ, this representation relates the two-point function of the field $\langle T\{\Psi(x)\Psi(0)\}\rangle$ to an integral convolution between the free field propagator and some spectral density ρ. The integral representation enables one to determine interesting information about the analytic structure of correlation functions, and also has many important applications including the establishment of Goldstone's theorem for relativistic local fields [76]. Another important result in quantum field theory (QFT) is the operator product expansion (OPE). This expansion was first proposed by Wilson [116] to describe the behaviour of products (or time-ordered products) of fields in the limit of coinciding space-time arguments. Given the renormalised fields $A(x)$ and $B(y)$, the OPE has the form:

$$A(x)B(y) \sim \sum_{i=1}^{n} \widetilde{C}_i(x-y)\widetilde{\mathcal{O}}_i(y) \tag{4.1}$$

where $\{\widetilde{\mathcal{O}}_i(y)\}_{i=1}^{n}$ is a finite set of renormalised fields, $\widetilde{C}_i$ are (possibly singular) coefficient functions, and $\sim$ is understood to imply that an insertion of $A(x)B(y) - \sum_{i=1}^{n} \widetilde{C}_i(x-y)\widetilde{\mathcal{O}}_i(y)$ into any Green's function will vanish in the (weak) limit $x \to y$. An important feature of the OPE is that both $\widetilde{\mathcal{O}}_i(y)$ and the coefficients $\widetilde{C}_i$ depend on an auxiliary parameter μ called the renormalisation scale. For the purpose of the discussions in this paper we are interested in the structure of two-point functions of certain fields Ψ. By using the general form of the OPE outlined in Eq. (4.1), these Green's functions can be shown to have the following behaviour in the limit $x \to 0$:

$$\langle T\{\Psi(x)\Psi(0)\}\rangle \sim \sum_{i} C_i(x)\langle\mathcal{O}_i(0)\rangle \tag{4.2}$$

where $\langle\cdot\rangle$ signifies the vacuum expectation value. The conceptual idea of the OPE is that the series provides an asymptotic decomposition of short and long distance degrees of freedom, which in the case of asymptotically free theories such as quantum chromodynamics (QCD) are partitioned between the Wilson coefficients $C_i(x)$ and vacuum condensates $\langle\mathcal{O}_i(0)\rangle$ respectively. For general theories though, this decomposition is not necessarily so clear-cut [118]. Nevertheless, the OPE has many important applications such as in the construction of factorisation theorems [45] and the calculation of conformal field theories [110], as well as more applied uses like in the determination of QCD observables such as R_{had} [128].

The spectral representation and the OPE are important results which have led to both successful experimental predictions and important theoretical developments. In particular, over the last few decades the determination of the perturbative and non-perturbative structure of QCD has significantly progressed due to the application of these results. The method that perhaps best epitomises the successful use of both the spectral representation and the OPE is the Shifman-Vainshtein-Zakharov (SVZ) sum rules [119]. By exploiting the analytic structure of certain correlation functions, this approach introduces a parametrised ansatz for the spectral density ρ and uses this to determine mesonic and hadronic parameters in terms of QCD vacuum condensates such as $\langle\bar{\psi}\psi\rangle$ and $\langle F^{a}_{\mu\nu}F^{a\mu\nu}\rangle$. Given lattice QCD estimates of these condensates, this then allows one to make a prediction for these parameters. The key point here is that it is not possible to exactly calculate the spectral density associated with a correlation function, the reason being that the complete analytic structure of QCD remains unknown. Instead, one has to constrain the form of ρ indirectly. Another example of a method which constrains the form of spectral densities is the so-called *Weinberg sum rules* [6]. These constraints are derived by performing a short distance expansion of the spectral representation of a correlation function, and inferring that certain linear combinations of the spectral densities must vanish if the correlation function in question has a specific singular behaviour.

It is clear that constraining the form of the spectral density is very important if one wants to improve understanding of QCD, as well as other QFTs. In the literature this problem has been pursued in a variety of different ways, the SVZ and the Weinberg sum rules being two of the more developed methods. An interesting approach adopted by [129] is to generalise the Weinberg sum rules by comparing the short distance spectral representation expansion of a correlator with its OPE. Based on which singular terms appear in the OPE, one can then conclude whether certain linear combinations of the spectral density vanish or not. In a similar manner, the authors in [118] compare the expression generated by the large momentum propagator expansion in ϕ^4-theory, with the leading singular terms in the OPE, but in this case with the intention of demonstrating the validity of the OPE itself. The success of this comparison approach between the short distance expanded spectral representation and the OPE, suggests that there may well be more information to be gained by performing a full expansion of both expressions, and then matching the resulting terms order by order in x.

The remainder of this paper is structured as follows: in Sec. 4.3 we perform the short distance matching procedure for the scalar propagator in ϕ^4-theory; in Sec. 4.4 we apply the same procedure to the quark propagator in QCD; and finally in Sec. 4.5 we discuss the relevance of our results and the scope for further applications.

4.3 Short distance matching in ϕ^4-theory

In this section the short distance matching procedure outlined at the end of Sec. 4.2 will be applied to the propagator $\langle T\{\phi(x)\phi(0)\}\rangle$ in ϕ^4 scalar field theory. Given the assumption of some standard QFT axioms[1], this propagator has the following spectral representation:

$$\langle T\{\phi(x)\phi(0)\}\rangle = \int_0^\infty ds\ \rho(s)\ i\Delta_F(x;s) \tag{4.3}$$

where $i\Delta_F(x;s)$ is the free bosonic Feynman propagator, and $\rho(s)$ is the spectral density. As with any QFT, renormalisation of the fields is required in order to remove the divergences which arise as a result of the product of fields being ill defined at coincident space-time points. Once this procedure has been performed, the propagator instead satisfies the following renormalised spectral representation [115]:

$$\langle T\{\phi_R(x)\phi_R(0)\}\rangle = \int_0^\infty ds\ \rho(s,\mu,g)\ i\Delta_F(x;s) \tag{4.4}$$

where ϕ_R is the renormalisation of the bare field ϕ, and the spectral density ρ is now also dependent on the renormalisation scale μ and coupling g. If one now assumes x to be space-like ($x^2 < 0$), the Lorentz invariance of the propagator enables one (for simplicity) to set $x_0 = 0$. Under these conditions the free boson propagator $i\Delta_F(x;s)$ has the following exact form [130]:

$$i\Delta_F(x_0 = 0, \mathbf{x}; s) = \frac{\sqrt{s}}{4\pi^2|\mathbf{x}|}K_1(\sqrt{s}|\mathbf{x}|) \tag{4.5}$$

where K_1 is a modified Bessel function of the second kind. Under the assumption that the small-$|\mathbf{x}|$ behaviour of the integral in Eq. (4.4) can be approximated by expanding the integrand around the point $|\mathbf{x}| = 0$, the propagator in this approximation is given by

$$\begin{aligned}\langle T\{\phi_R(x)\phi_R(0)\}\rangle \sim \int_0^\infty ds\ \rho(s,\mu,g)\Bigg[\frac{s}{16\pi^2}\left[2\gamma - 1 + 2\ \ln\left(\frac{\sqrt{s}}{2}\right) + 2\ \ln\left(|\mathbf{x}|\right)\right] \\ + \frac{1}{4\pi^2|\mathbf{x}|^2} + \mathcal{O}(|\mathbf{x}|^2)\Bigg]\end{aligned} \tag{4.6}$$

[1] See [111–114] for more details.

Moreover, the renormalised propagator also has the following OPE [117]:

$$\langle T\{\phi_R(x)\phi_R(0)\}\rangle \sim C_{\mathbb{I}}(x,\mu,m,g) + C_{\phi^2}(x,\mu,m,g)\langle\phi_R^2(0)\rangle + \cdots \tag{4.7}$$

where m is the renormalised mass parameter, $\phi_R^2 = [\phi^2]_R$ is the renormalisation of the bare field ϕ^2, and $\cdots$ represents other possible non-singular terms. Under the assumption that x is space-like (with $x_0 = 0$), this asymptotic expansion is valid in the limit $|\mathbf{x}| \to 0$. The Wilson coefficients $C_{\mathbb{I}}$ and C_{ϕ^2} can be calculated perturbatively, and it turns out that to lowest order in perturbation theory they have the following form [131]:

$$C_{\mathbb{I}}(x,\mu,m,g) = \frac{1}{4\pi^2|\mathbf{x}|^2} + \frac{m^2}{16\pi^2}\ln\left(\mu^2|\mathbf{x}|^2\right) + \mathcal{O}(g^2) \tag{4.8}$$

$$C_{\phi^2}(x,\mu,m,g) = 1 + \frac{g}{32\pi^2}\ln\left(\mu^2|\mathbf{x}|^2\right) + \mathcal{O}(g^2) \tag{4.9}$$

Inserting these expressions into Eq. (4.7) then gives

$$\begin{aligned}\langle T\{\phi_R(x)\phi_R(0)\}\rangle \sim \frac{1}{4\pi^2|\mathbf{x}|^2} + \frac{m^2}{16\pi^2}\ln\left(\mu^2|\mathbf{x}|^2\right) + \langle\phi_R^2(0)\rangle \\ + \frac{g}{32\pi^2}\ln\left(\mu^2|\mathbf{x}|^2\right)\langle\phi_R^2(0)\rangle + \mathcal{O}(g^2)\end{aligned} \tag{4.10}$$

Since Eqs. (4.6) and (4.10) correspond to equivalent descriptions of the propagator in the small-$|\mathbf{x}|$ limit, and the spectral density ρ is not x dependent, one can equate these two equations and match the coefficients of the various $|\mathbf{x}|$-dependent terms. In doing so, one obtains the following relations between the OPE coefficients and certain moments of the spectral density:

$$\mathcal{O}\left(\tfrac{1}{|\mathbf{x}|^2}\right): \int_0^\infty ds\ \rho(s,\mu,g) = 1 \tag{4.11}$$

$$\begin{aligned}\mathcal{O}\left(|\mathbf{x}|^0\right): \int_0^\infty ds\ s\rho(s,\mu,g)\left[2\gamma - 1 + 2\ \ln\left(\frac{\sqrt{s}}{2}\right)\right] = 2m^2\ln(\mu) + 16\pi^2\langle\phi_R^2(0)\rangle \\ + g\ln(\mu)\langle\phi_R^2(0)\rangle + \mathcal{O}(g^2)\end{aligned} \tag{4.12}$$

$$\mathcal{O}\left(\ln(|\mathbf{x}|)\right): \int_0^\infty ds\ s\rho(s,\mu,g) = m^2 + \frac{g}{2}\langle\phi_R^2(0)\rangle + \mathcal{O}(g^2) \tag{4.13}$$

One thing to notice here is that the relation in Eq. (4.11) is exact since there are no other $\mathcal{O}\left(\frac{1}{|\mathbf{x}|^2}\right)$ terms in Eq. (4.6), and it is not possible to generate another term with this dependence in Eq. (4.10) no matter what perturbative order C_{ϕ^2} and $C_{\mathbb{I}}$ are expanded to. Equations (4.12)–(4.13) on the other hand are only perturbatively valid to $\mathcal{O}(g^2)$, since expanding C_{ϕ^2} and $C_{\mathbb{I}}$ to higher orders may generate additional constant or $\mathcal{O}\left(\ln\left(|\mathbf{x}|\right)\right)$ terms. By inspecting Eq. (4.13), it is clear that this is satisfied if the spectral density is given by

$$\rho(s,\mu,g) = \delta(s-m^2) + \frac{g}{2}\langle\phi_R^2(0)\rangle A(s) + \mathcal{O}(g^2) \tag{4.14}$$

where $A(s)$ satisfies the normalisation condition

$$\int_0^\infty ds\ sA(s) = 1 \tag{4.15}$$

and also implicitly depends on the renormalisation scale μ. From Eq. (4.14) one can see that the spectral density has several interesting features: there is a Dirac delta term which corresponds to the existence of a state with mass m in the theory; the second term has the structure of a continuum component since it contains an explicit factor of the coupling constant g, and is hence a by-product of interactions in the theory; and also the second term is premultiplied by the condensate $\langle\phi_R^2(0)\rangle$, which suggests that the contribution of this continuum component to the spectral density is moderated by the magnitude of the scalar condensate.

Inserting this expression for the spectral density into Eq. (4.12), and ignoring terms of $\mathcal{O}(g^2)$ and above, one obtains the relation

$$\begin{aligned}\frac{g}{2}\langle\phi_R^2(0)\rangle\left[2\gamma-\ln(4)-1+\mathcal{I}\right]+m^2\left[2\gamma-1+2\ \ln\left(\frac{m}{2}\right)\right] &= 2m^2\ln(\mu)+16\pi^2\langle\phi_R^2(0)\rangle \\ &\quad + g\ln(\mu)\langle\phi_R^2(0)\rangle+\mathcal{O}(g^2)\end{aligned} \tag{4.16}$$

where $\mathcal{I}$ has the form

$$\mathcal{I} = \int_0^\infty ds\ s\ln(s)A(s) \tag{4.17}$$

Upon rearrangement this gives

$$\begin{aligned}\langle\phi_R^2(0)\rangle &= \left(1+\frac{g}{16\pi^2}\mathcal{I}'\right)^{-1}\left[\mathcal{C}-\frac{m^2}{8\pi^2}\ln\left(\frac{\mu}{m}\right)\right]+\mathcal{O}(g^2) \\ &= \mathcal{C}-\frac{m^2}{8\pi^2}\ln\left(\frac{\mu}{m}\right)-\frac{g}{16\pi^2}\mathcal{I}'\mathcal{C}+\frac{gm^2}{128\pi^4}\ln\left(\frac{\mu}{m}\right)\mathcal{I}'+\mathcal{O}(g^2)\end{aligned} \tag{4.18}$$

where $\mathcal{I}'$ and $\mathcal{C}$ are

$$\mathcal{I}' = \ln(\mu) - \frac{1}{2}\left[2\gamma - \ln(4) - 1 + \mathcal{I}\right] \tag{4.19}$$

$$\mathcal{C} = \frac{m^2}{16\pi^2}\left[2\gamma - \ln(4) - 1\right] \tag{4.20}$$

A significant feature of the expression for the condensate in Eq. (4.18) is that it explicitly depends on $\mathcal{I}$, an integral involving the *a priori* unknown continuum contribution to the spectral density $A(s)$. Because this condensate does not receive any non-perturbative contributions [118], it must have exactly the same form as the purely perturbative expression for $\langle\phi_R^2(0)\rangle$ computed using the renormalisation of the operator $\phi^2(0)$. Therefore, by equating these expressions one can obtain information about the continuum component $A(s)$.

In general, a renormalised operator $\mathcal{O}_R^i$ satisfies the following renormalisation group equation (RGE) [117]:

$$\mu\frac{d}{d\mu}\mathcal{O}_R^i = \sum_j \gamma_{ij}\mathcal{O}_R^j \tag{4.21}$$

where γ_{ij} is the anomalous dimension matrix and $\{\mathcal{O}_R^j\}$ is a finite closed basis of renormalised operators with dimension $\leq \dim(\mathcal{O}_R^i)$. In ϕ^4-theory $\phi_R^2(0)$ mixes with the identity operator $\mathbb{I}$, but not with $\phi_R(0)$ [117]. The RGE for $\phi_R^2(0)$ therefore has the form

$$\mu\frac{d}{d\mu}\phi_R^2(0) = \sum_j \gamma_{\phi^2 j}\mathcal{O}_R^j = \gamma_{\phi^2\phi^2}\phi_R^2(0) + \gamma_{\phi^2\mathbb{I}}\mathbb{I} \tag{4.22}$$

By definition, the vacuum expectation value of $\phi_R^2(0)$ with the perturbative (Fock space) vacuum state vanishes. However, the vacuum expectation value with the physical non-perturbative vacuum state does not necessarily vanish, and this is what $\langle\phi_R^2(0)\rangle$ corresponds to both in the preceding and proceeding discussions in this section. After inserting both sides of Eq. (4.22) between the physical vacuum state, one obtains the following RGE for $\langle\phi_R^2(0)\rangle$:

$$\left(\mu\frac{d}{d\mu} - \gamma_{\phi^2\phi^2}\right)\langle\phi_R^2(0)\rangle = \left(\mu\frac{\partial}{\partial\mu} + \beta\frac{\partial}{\partial g} + \gamma_m m\frac{\partial}{\partial m} - \gamma_{\phi^2\phi^2}\right)\langle\phi_R^2(0)\rangle = \gamma_{\phi^2\mathbb{I}} \tag{4.23}$$

where β is the beta function of the theory and γ_m is the anomalous mass dimension[2]. At one-loop order one has [131, 132]

$$\beta = \frac{3g^2}{16\pi^2}, \quad \gamma_{\phi^2\phi^2} = -2\gamma_m = -\frac{g}{16\pi^2}, \quad \gamma_{\phi^2\mathbb{I}} = -\frac{m^2}{8\pi^2} \tag{4.24}$$

By choosing a mass-independent renormalised operator basis, in this case $\{\mathbb{I}, \phi_R^2\}$, the anomalous dimensions can in general become mass dependent [117], and this is in fact what happens for $\gamma_{\phi^2\mathbb{I}}$. Using the method of characteristics, the solution of Eq. (4.23) is equivalent to the solution of the following set of ordinary differential equations:

$$\frac{d\ln\mu}{dt} = 1 \tag{4.25}$$

$$\frac{dg}{dt} = \beta = \frac{3g^2}{16\pi^2} \tag{4.26}$$

$$\frac{dm}{dt} = \gamma_m m = \frac{gm}{32\pi^2} \tag{4.27}$$

$$\frac{d}{dt}\langle\phi_R^2(0)\rangle = \gamma_{\phi^2\phi^2}\langle\phi_R^2(0)\rangle + \gamma_{\phi^2\mathbb{I}} = -\frac{g}{16\pi^2}\langle\phi_R^2(0)\rangle - \frac{m^2}{8\pi^2} \tag{4.28}$$

However, in order to obtain unique solutions one must first specify a boundary condition for each equation. Since the variable t has no physical significance and only serves to parametrise the characteristic curves along which solutions are defined, one can choose all of the boundary data to be at $t = 0$. For Eq. (4.25) the general solution is given by $\ln\mu = t + c_1$, so the integration constant has the form $c_1 = \ln\mu(t = 0)$. Letting $c_1 = \ln(\bar{\mu})$, where $\bar{\mu}$ is some physical scale, the condition $t = 0$ is equivalent to $\mu = \bar{\mu}$, and so $t = \ln\left(\frac{\mu}{\bar{\mu}}\right)$. With this choice of boundary condition the solutions of Eqs. (4.26)–(4.27) can be written

$$g = \bar{g}\left(1 - \frac{3\bar{g}t}{16\pi^2}\right)^{-1} \qquad m = \overline{m}\left(1 - \frac{3\bar{g}t}{16\pi^2}\right)^{-\frac{1}{6}} \tag{4.29}$$

where $\bar{g} = g(t = 0)$, $\overline{m} = m(t = 0)$, and the solution of $\langle\phi_R^2(0)\rangle$ has the form

$$\langle\phi_R^2(0)\rangle = \frac{2\overline{m}^2}{\bar{g}}\left(1 - \frac{3\bar{g}t}{16\pi^2}\right)^{\frac{2}{3}} - \frac{2\overline{m}^2}{\bar{g}}\left(1 - \frac{3\bar{g}t}{16\pi^2}\right)^{\frac{1}{3}} + \overline{\langle\phi_R^2(0)\rangle}\left(1 - \frac{3\bar{g}t}{16\pi^2}\right)^{\frac{1}{3}} \tag{4.30}$$

with $\overline{\langle\phi_R^2(0)\rangle} = \langle\phi_R^2(0)\rangle(t = 0)$. By inverting the expressions in Eq. (4.29), one can rewrite the solution in Eq. (4.30) exclusively in terms of the parameters g, m and

[2] Here we use the opposite sign convention to [132] for γ_m.

$t = \ln\left(\frac{\mu}{\bar{\mu}}\right)$. Doing so gives

$$\langle\phi_R^2(0)\rangle = \frac{2m^2}{g} + \overline{\langle\phi_R^2(0)\rangle}\left[1 + \frac{3g}{16\pi^2}\ln\left(\frac{\mu}{\bar{\mu}}\right)\right]^{-\frac{1}{3}} - \frac{2m^2}{g}\left[1 + \frac{3g}{16\pi^2}\ln\left(\frac{\mu}{\bar{\mu}}\right)\right]^{\frac{1}{3}} \quad (4.31)$$

Because this perturbative determination of $\langle\phi_R^2(0)\rangle$ is valid up to one-loop order, the solution is therefore equal to the following expansion of Eq. (4.31) up to $\mathcal{O}(g)$:

$$\langle\phi_R^2(0)\rangle = \overline{\langle\phi_R^2(0)\rangle} - \frac{m^2}{8\pi^2}\ln\left(\frac{\mu}{\bar{\mu}}\right) - \frac{g}{16\pi^2}\ \ln\left(\frac{\mu}{\bar{\mu}}\right)\overline{\langle\phi_R^2(0)\rangle} + \frac{gm^2}{128\pi^4}\left[\ln\left(\frac{\mu}{\bar{\mu}}\right)\right]^2 + \mathcal{O}(g^2) \quad (4.32)$$

Finally, one can now compare this equation with the expression for $\langle\phi_R^2(0)\rangle$ [(Eq. (4.18)] obtained via the spectral density matching conditions in Eqs. (4.11)–(4.13). One can clearly see that these expressions have a very similar form. In fact, using the solutions for g and m, one can rewrite Eq. (4.18) as follows:

$$\begin{aligned}\langle\phi_R^2(0)\rangle = \widetilde{\mathcal{C}} - \frac{m^2}{8\pi^2}\ln\left(\frac{\mu}{\overline{m}}\right) + \frac{g}{16\pi^2}\widetilde{\mathcal{C}}\ \ln\left(\frac{\mu}{\bar{\mu}}\right) + \frac{gm^2}{256\pi^4}\ln\left(\frac{\mu}{\bar{\mu}}\right) \\ - \frac{g}{16\pi^2}\mathcal{I}'\widetilde{\mathcal{C}} + \frac{gm^2}{128\pi^4}\ln\left(\frac{\mu}{\overline{m}}\right)\mathcal{I}' + \mathcal{O}(g^2)\end{aligned} \quad (4.33)$$

where the constant $\widetilde{\mathcal{C}}$ is defined as

$$\widetilde{\mathcal{C}} = \frac{\overline{m}^2}{16\pi^2}\left[2\gamma - \ln(4) - 1\right] \quad (4.34)$$

By demanding that $\mathcal{I}'$ satisfies the following relation

$$\mathcal{I}' = \ln\left(\frac{\mu}{\overline{m}}\right) + \frac{2\ln\left(\frac{\mu}{\overline{m}}\right)\left[\gamma - \ln(2)\right]}{\left[\left[2\gamma - \ln(4) - 1\right] - 2\ln\left(\frac{\mu}{\overline{m}}\right)\right]} \quad (4.35)$$

the expression for $\langle\phi_R^2(0)\rangle$ becomes

$$\langle\phi_R^2(0)\rangle = \widetilde{\mathcal{C}} - \frac{m^2}{8\pi^2}\ln\left(\frac{\mu}{\overline{m}}\right) - \frac{g}{16\pi^2}\ln\left(\frac{\mu}{\overline{m}}\right)\widetilde{\mathcal{C}} + \frac{gm^2}{128\pi^4}\left[\ln\left(\frac{\mu}{\overline{m}}\right)\right]^2 + \mathcal{O}(g^2) \quad (4.36)$$

which has exactly the same form as Eq. (4.32) if one makes the identification

$$\bar{\mu} = \overline{m}, \qquad \overline{\langle\phi_R^2(0)\rangle} = \widetilde{\mathcal{C}} \quad (4.37)$$

So equating the short distance matched and RGE derived expressions for $\langle \phi_R^2(0) \rangle$ has introduced two new constraints: the functional form of the initial conditions in Eqs. (4.25)–(4.28) is fixed, and hence the form of $\langle \phi_R^2(0) \rangle$ is completely specified in terms of the free parameters $\overline{m}$ and $\bar{g}$; and the condition in Eq. (4.35) implies that $A(s)$ must satisfy

$$\int_0^\infty ds\ s\ \ln(s) A(s) = \ln(4\overline{m}^2) - 2\gamma + 1 - \frac{4\ln\left(\frac{\mu}{\overline{m}}\right)\left[\gamma - \ln(2)\right]}{\left[\left[2\gamma - \ln(4) - 1\right] - 2\ln\left(\frac{\mu}{\overline{m}}\right)\right]} \tag{4.38}$$

and therefore provides an additional constraint on the form of the spectral density ρ.

Although ϕ^4-theory may well not be physically realistic due to its triviality [47, 55], the discussion in this section demonstrates that the short distance matching procedure provides a way of determining new constraints and qualitative features of the theory, and in particular the spectral density, which contrasts with numerical-based approaches [133–135]. Moreover, because this procedure is model independent, since it only relies on the existence of an OPE and a spectral representation, it can also equally be applied to physically realistic theories such as QCD, and this is what we pursue in Sec. 4.4.

4.4 Short distance matching in QCD

The short distance matching procedure that was performed for ϕ^4-theory is equally applicable to QCD, and in this section we focus in particular on analysing the fermionic quark propagator $\langle T\{\psi(x)\overline{\psi}(0)\}\rangle$ in this way. For this propagator, the spectral density ρ can be decomposed in spinor space as [136]

$$\rho(s) = \rho_S(s)\mathbb{I} + \rho_{PS}(s)\gamma_5 + \rho_V^\mu(s)\gamma_\mu + \rho_{PV}^\mu(s)\gamma_5\gamma_\mu + \rho_T^{\mu\nu}(s)\sigma_{\mu\nu} \tag{4.39}$$

where the spinor indices are suppressed. It turns out that the tensor term in Eq. (4.39) does not contribute, and furthermore if one assumes the absence of parity violation, then $\rho_{PS} = \rho_{PV} = 0$. Combining these results, the quark propagator has the following renormalised spectral representation:

$$\langle T\{\psi_R(x)\overline{\psi}_R(0)\}\rangle = \int_0^\infty ds\ \rho_V(s,\mu,g)\ iS_F(x;s) + i\Delta_F(x;s)\Big[\rho_S(s,\mu,g) - \sqrt{s}\,\rho_V(s,\mu,g)\Big] \tag{4.40}$$

where $i\Delta_F(x;s)$ and $iS_F(x;s)$ are the free bosonic and fermionic Feynman propagators respectively, $\rho_V^\mu(s=p^2) := p^\mu \rho_V(s)$, and ψ_R, $\overline{\psi}_R$ are the renormalised bare fields. Assuming x is space-like (and setting $x_0 = 0$), one can perform a small-$|\mathbf{x}|$ expansion in an analogous way to Sec. 4.3. The space-like structure of the free bosonic propagator is given by Eq. (4.5), and for the free fermionic propagator it has the form

$$\begin{aligned} iS_F(x_0=0,\mathbf{x};s) &= \left[\left(i\partial\!\!\!/ + \sqrt{s}\right) i\Delta_F(x;s)\right]_{x_0=0} \\ &= -i\gamma^i x_i \left[\frac{s\left[K_0(\sqrt{s}|\mathbf{x}|) + K_2(\sqrt{s}|\mathbf{x}|)\right]}{8\pi^2|\mathbf{x}|^2} + \frac{\sqrt{s}}{4\pi^2|\mathbf{x}|^3} K_1(\sqrt{s}|\mathbf{x}|)\right] \\ &\quad + \frac{s}{4\pi^2|\mathbf{x}|} K_1(\sqrt{s}|\mathbf{x}|) \end{aligned} \tag{4.41}$$

Finally, inserting the explicit expressions for the free propagators into Eq. (4.40), and expanding around the point $|\mathbf{x}| = 0$, one obtains

$$\begin{aligned} \langle T\{\psi_R(x)\overline{\psi}_R(0)\}\rangle \sim \int_0^\infty ds\ \rho_V(s,\mu,g) &\left[-\frac{i\cancel{\mathbf{x}}}{2\pi^2|\mathbf{x}|^4} + \frac{is\cancel{\mathbf{x}}}{8\pi^2|\mathbf{x}|^2} + \mathcal{O}(|\cancel{\mathbf{x}}|)\right] \\ + \rho_S(s,\mu,g) &\left[\frac{s}{16\pi^2}\left[2\ \ln\left(\frac{\sqrt{s}}{2}\right) + 2\gamma - 1 + 2\ \ln(|\mathbf{x}|)\right]\right. \\ &\left. + \frac{1}{4\pi^2|\mathbf{x}|^2} + \mathcal{O}(|\mathbf{x}|^2)\right] \end{aligned} \tag{4.42}$$

In a similar manner to ϕ^4-theory, the quark propagator[3] has the following operator product expansion [37]:

$$\langle T\{\psi_R(x)\overline{\psi}_R(0)\}\rangle \sim C_{\mathbb{I}}(x,\mu,m,g) + C_{\overline{\psi}\psi}(x,\mu,m,g)\langle\overline{\psi}\psi(0)\rangle + \cdots \tag{4.43}$$

where $C_{\mathbb{I}}$ and $C_{\overline{\psi}\psi}$ satisfy the RGEs

$$\mu\frac{d}{d\mu}C_{\overline{\psi}\psi} = -\gamma_{\overline{\psi}\psi,\overline{\psi}\psi}C_{\overline{\psi}\psi} \qquad \mu\frac{d}{d\mu}C_{\mathbb{I}} = -\gamma_{\overline{\psi}\psi,\mathbb{I}}C_{\overline{\psi}\psi} \tag{4.44}$$

[3]For simplicity we assume here that there is only one flavour of quark, with mass m.

With this RGE convention for the Wilson coefficients, the anomalous dimensions at one-loop order are given by [137][4]

$$\gamma_{\bar{\psi}\psi,\bar{\psi}\psi} = \frac{g^2}{2\pi^2}, \qquad \gamma_{\bar{\psi}\psi,\mathbb{I}} = \frac{3m^3}{2\pi^2}\left(1 + \frac{g^2}{3\pi^2}\right) \tag{4.45}$$

Just like in Sec. 4.3, one can solve these equations using the method of characteristics. In this case, solving these equations (to one-loop order) requires one to solve the following ordinary differential equations:

$$\begin{aligned}
\frac{d\ln\mu}{dt} &= 1 && (4.46)\\
\frac{dg}{dt} &= \beta = -\frac{7g^3}{16\pi^2} && (4.47)\\
\frac{dm}{dt} &= \gamma_m m = -\frac{g^2 m}{2\pi^2} && (4.48)\\
\frac{d}{dt}C_{\bar{\psi}\psi} &= -\frac{g^2}{2\pi^2}C_{\bar{\psi}\psi} && (4.49)\\
\frac{d}{dt}C_{\mathbb{I}} &= -\frac{3m^3}{2\pi^2}\left(1 + \frac{g^2}{3\pi^2}\right)C_{\bar{\psi}\psi} && (4.50)
\end{aligned}$$

With the initial conditions $\mu(t=0) = \frac{1}{|\mathbf{x}|}$, $g(t=0) = \bar{g}$, and $m(t=0) = \overline{m}$, one has

$$g^2 = \bar{g}^2\left(1 + \frac{7\bar{g}^2 t}{8\pi^2}\right)^{-1} \qquad m = \overline{m}\left(1 + \frac{7\bar{g}^2 t}{8\pi^2}\right)^{-\frac{4}{7}} \tag{4.51}$$

where $t = \ln(\mu|\mathbf{x}|)$, and the Wilson coefficients have the following form:

$$C_{\bar{\psi}\psi} = -\left(1 - \frac{7g^2 t}{8\pi^2}\right)^{\frac{4}{7}} \tag{4.52}$$

$$\begin{aligned}
C_{\mathbb{I}} = &-\frac{i\not{\mathbf{x}}}{2\pi^2|\mathbf{x}|^4} + \frac{m}{4\pi^2|\mathbf{x}|^2} + \frac{i\not{\mathbf{x}}m^2}{8\pi^2|\mathbf{x}|^2} + \frac{4m^3}{3g^2}\left[1 + \frac{3g^2}{16\pi^2}\left(1 - \frac{7g^2 t}{8\pi^2}\right)^{-1}\right]\left(1 - \frac{7g^2 t}{8\pi^2}\right)^{-\frac{5}{7}}\\
&- \frac{4m^3}{3g^2}\left[1 + \frac{g^2}{16\pi^2}(3 + 14t)\left(1 - \frac{7g^2 t}{8\pi^2}\right)^{-1}\right]\left(1 - \frac{7g^2 t}{8\pi^2}\right)^{\frac{11}{7}}
\end{aligned} \tag{4.53}$$

[4] As in Sec. 4.3, we adopt a mass-independent renormalised operator basis here (like [37]), which means that the anomalous dimensions can in general be mass dependent, unlike in [137]. Nevertheless, the mass-dependent anomalous dimensions are related to the mass-independent ones by a multiplication of a certain power in the mass m (in this case $\gamma_{\bar{\psi}\psi,\mathbb{I}} = m^3\gamma_{\bar{\psi}\psi,m^3}$), and these choices lead to the same RGE for $\bar{\psi}\psi(0)$.

Expanding these expressions to $\mathcal{O}(g^2)$ and inserting them into Eq. (4.43) gives

$$\begin{aligned}\langle T\{\psi_R(x)\overline{\psi}_R(0)\}\rangle \sim &- \frac{i\not{x}}{2\pi^2|\mathbf{x}|^4} + \frac{m}{4\pi^2|\mathbf{x}|^2} + \frac{i\not{x}m^2}{8\pi^2|\mathbf{x}|^2} + \frac{3m^3}{2\pi^2}\ln(\mu|\mathbf{x}|) + \frac{g^2m^3}{2\pi^4}\ln(\mu|\mathbf{x}|) \\ &+ \frac{3g^2m^3}{4\pi^4}\left[\ln(\mu|\mathbf{x}|)\right]^2 - \langle\overline{\psi}\psi(0)\rangle + \frac{g^2}{2\pi^2}\ln(\mu|\mathbf{x}|)\langle\overline{\psi}\psi(0)\rangle + \mathcal{O}(g^3)\end{aligned} \tag{4.54}$$

Since both the spectral densities are x independent, one can perform the same procedure as in Sec. 4.3, and match the different $|\mathbf{x}|$-dependent coefficients in this expression with the moments of the spectral density in Eq. 4.42:

$$\mathcal{O}\left(\tfrac{\not{x}}{|\mathbf{x}|^4}\right): \int_0^\infty ds\ \rho_V(s,\mu,g) = 1 \tag{4.55}$$

$$\mathcal{O}\left(\tfrac{1}{|\mathbf{x}|^2}\right): \int_0^\infty ds\ \rho_S(s,\mu,g) = m \tag{4.56}$$

$$\mathcal{O}\left(\tfrac{\not{x}}{|\mathbf{x}|^2}\right): \int_0^\infty ds\ s\rho_V(s,\mu,g) = m^2 \tag{4.57}$$

$$\begin{aligned}\mathcal{O}\left(|\mathbf{x}|^0\right): \int_0^\infty ds\ s\rho_S(s,\mu,g)\left[2\gamma - 1 + 2\ \ln\left(\frac{\sqrt{s}}{2}\right)\right] &= 24m^3\ln(\mu) + \frac{8g^2m^3}{\pi^2}\ln(\mu) \\ &+ \frac{12g^2m^3}{\pi^2}\left[\ln(\mu)\right]^2 - 16\pi^2\langle\overline{\psi}\psi(0)\rangle \\ &+ 8g^2\ln(\mu)\langle\overline{\psi}\psi(0)\rangle + \mathcal{O}(g^3)\end{aligned} \tag{4.58}$$

$$\mathcal{O}\left(\ln(|\mathbf{x}|)\right): \int_0^\infty ds\ s\rho_S(s,\mu,g) = 12m^3 + \frac{4g^2m^3}{\pi^2} + \frac{12g^2m^3}{\pi^2}\ln(\mu) + 4g^2\langle\overline{\psi}\psi(0)\rangle + \mathcal{O}(g^3) \tag{4.59}$$

From Eq. (4.59) one can see that this relation is satisfied if the scalar spectral density has the following form:

$$\rho_S(s,\mu,g) = \left[12 + \frac{4g^2}{\pi^2} + \frac{12g^2}{\pi^2}\ln(\mu)\right] m\,\delta(s-m^2) + 4g^2\langle\overline{\psi}\psi(0)\rangle B(s) + \mathcal{O}(g^3) \tag{4.60}$$

where $B(s)$ satisfies the normalisation constraint

$$\int_0^\infty ds\ sB(s) = 1 \tag{4.61}$$

and also implicitly depends on the renormalisation scale μ. It is interesting to note here that ρ_S has the same characteristics as the ϕ^4 spectral density in Eq. (4.14): a Dirac delta term, and a continuum contribution $B(s)$ which has an explicit coupling constant and condensate prefactor.

Similarly to Sec. 4.3, by substituting ρ_S into Eq. (4.58) one can rearrange to obtain an explicit expression for the quark condensate:

$$\begin{aligned}\langle\bar{\psi}\psi(0)\rangle = \mathcal{K} + \frac{3m^3}{2\pi^2}\ln\left(\frac{\mu}{m}\right) + \frac{g^2m^3}{2\pi^4}\ln\left(\frac{\mu}{m}\right) + \frac{g^2}{2\pi^2}\mathcal{J}'\mathcal{K} + \frac{3g^2m^3}{4\pi^4}\ln\left(\frac{\mu}{m}\right)\mathcal{J}' \\ + \frac{3g^2m^3}{4\pi^4}\Big[[\ln(\mu)]^2 - 2\ln(m)\ln(\mu)\Big] + \mathcal{K}\left[\frac{g^2}{3\pi^2} + \frac{g^2}{\pi^2}\ln(\mu)\right] + \mathcal{O}(g^3)\end{aligned} \tag{4.62}$$

where $\mathcal{K}$ and $\mathcal{J}'$ are given by

$$\mathcal{J}' = \ln(\mu) - \frac{1}{2}\left[2\gamma - \ln(4) - 1 + \mathcal{J}\right] \tag{4.63}$$

$$\mathcal{K} = -\frac{3m^3}{4\pi^2}\left[2\gamma - \ln(4) - 1\right] \tag{4.64}$$

and $\mathcal{J}$ is defined as

$$\mathcal{J} = \int_0^\infty ds\; s\ln(s)\, B(s) \tag{4.65}$$

In just the same way, this condensate explicitly depends on the unknown continuum component of the spectral density $B(s)$. However, unlike the scalar condensate in ϕ^4-theory, $\langle\bar{\psi}\psi(0)\rangle$ contains both perturbative *and* non-perturbative contributions [138], and as we demonstrate it turns out that the non-perturbative contributions arise due to $B(s)$. To make this more precise, one must first calculate the perturbative contributions to $\langle\bar{\psi}\psi(0)\rangle$ [denoted $\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}}$] which originate from the renormalisation of $\bar{\psi}\psi$. The RGE of $\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}}$ is

$$\mu\frac{d}{d\mu}\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}} = \gamma_{\bar{\psi}\psi,\bar{\psi}\psi}\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}} + \gamma_{\bar{\psi}\psi,\mathbb{I}} \tag{4.66}$$

where $\gamma_{\bar{\psi}\psi,\bar{\psi}\psi}$ and $\gamma_{\bar{\psi}\psi,\mathbb{I}}$ are given in Eq. (4.45). With the boundary condition $\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}}(t =$

$0) = \overline{\langle\bar{\psi}\psi(0)\rangle}_{\mathrm{P}}$, the solution to Eq. (4.66) has the form

$$\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}} = \frac{4m^3}{3g^2}\left[1+\frac{3g^2}{16\pi^2}\left(1-\frac{7g^2t}{8\pi^2}\right)^{-1}\right]\left(1-\frac{7g^2t}{8\pi^2}\right)^{-\frac{9}{7}} + \overline{\langle\bar{\psi}\psi(0)\rangle}_{\mathrm{P}}\left(1-\frac{7g^2t}{8\pi^2}\right)^{-\frac{4}{7}}$$
$$- \frac{4m^3}{3g^2}\left[1+\frac{g^2}{16\pi^2}(3+14t)\left(1-\frac{7g^2t}{8\pi^2}\right)^{-1}\right]\left(1-\frac{7g^2t}{8\pi^2}\right) \tag{4.67}$$

Because the anomalous dimensions used in Eq. (4.66) are only valid up to $\mathcal{O}(g^2)$, the perturbative expansion of $\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}}$ is also only valid up to this order. Performing this expansion gives

$$\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}} = \overline{\langle\bar{\psi}\psi(0)\rangle}_{\mathrm{P}} + \frac{3m^3}{2\pi^2}\ln\left(\frac{\mu}{\bar{\mu}}\right) + \frac{g^2m^3}{2\pi^4}\ln\left(\frac{\mu}{\bar{\mu}}\right)$$
$$+ \frac{g^2}{2\pi^2}\ln\left(\frac{\mu}{\bar{\mu}}\right)\overline{\langle\bar{\psi}\psi(0)\rangle}_{\mathrm{P}} + \frac{3g^2m^3}{2\pi^4}\left[\ln\left(\frac{\mu}{\bar{\mu}}\right)\right]^2 + \mathcal{O}(g^3) \tag{4.68}$$

By also expanding Eq. (4.62) to $\mathcal{O}(g^2)$, and comparing this expression with Eq. (4.68), the quark condensate can be decomposed as follows:

$$\langle\bar{\psi}\psi(0)\rangle = \langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}} + \frac{g^2}{2\pi^2}\left[\widetilde{\mathcal{K}} + \frac{3\overline{m}^3}{2\pi^2}\ln\left(\frac{\mu}{\overline{m}}\right)\right]\Bigg[\ln(2\overline{m}) - \gamma + \frac{1}{2}(1-\mathcal{J})$$
$$+ \frac{2\left[\ln(\overline{m})\right]^2 - \left[2\gamma - \ln(4) - 1\right]\left[3\ln\left(\frac{\mu}{\overline{m}}\right) - \frac{2}{3} - 2\ln(\mu)\right] - 2}{\left[\left[2\gamma - \ln(4) - 1\right] - 2\ln\left(\frac{\mu}{\overline{m}}\right)\right]}\Bigg] \tag{4.69}$$

where $\bar{\mu} = \overline{m}$ and $\langle\bar{\psi}\psi(0)\rangle_{\mathrm{P}}$ has the form of Eq. (4.68) with

$$\overline{\langle\bar{\psi}\psi(0)\rangle}_{\mathrm{P}} = \widetilde{\mathcal{K}} = -\frac{3\overline{m}^3}{4\pi^2}\left[2\gamma - \ln(4) - 1\right] \tag{4.70}$$

Since the first term is purely perturbative, it must be the case that the second term parametrises the non-perturbative contributions to the quark condensate, and in particular, the integral $\mathcal{J}$ involving $B(s)$. This explicit decomposition of the quark condensate into perturbative and non-perturbative contributions has not to our knowledge been established before in the literature, and instead has simply been assumed [138]. Moreover, the direct connection between the non-perturbative contributions and the continuum component of the scalar spectral density $B(s)$ has not been made before.

This has interesting applications because it means that if one can estimate the form of $B(s)$ from the integral constraints in Eqs. (4.56), (4.58) and (4.61), one can use Eq. (4.69) to directly estimate the non-perturbative component of $\langle\bar{\psi}\psi(0)\rangle$.

The analysis in this section has demonstrated that by equating the short distance expansion of the spectral representation of the quark propagator in QCD with its OPE, one can obtain novel information. A nice feature of this method, by contrast to more numerical-based approaches [126, 139, 140], is that it requires practically no theoretical input other than the form of the Wilson coefficients, and yet from this one is able to derive the qualitative structure of the scalar spectral density ρ_S, impose integral constraints on both ρ_S and ρ_V, and explicitly decompose the perturbative and non-perturbative contributions to $\langle\bar{\psi}\psi(0)\rangle$. Moreover, unlike techniques such as the SVZ sum rules, phenomenological approximations such as quark-hadron duality [141] are not assumed, which makes this approach process independent and therefore applicable to arbitrary correlators. In principle, this approach could also provide useful input for the SVZ sum rules. A key feature of these sum rules is the requirement to introduce a parametrised form of a spectral density [121], and so information obtained about the structure of this spectral density from the short distance matching procedure could be used to provide additional constraints on the corresponding parameters.

4.5 Conclusions

Spectral densities play a central role in determining the dynamics of a QFT, and yet in many instances it is not possible to calculate these objects exactly. This obstruction arises because the non-perturbative structure of these theories is not well understood. Nevertheless, one can infer information about the form of spectral densities by applying general QFT techniques. In particular, in this paper we have demonstrated that by matching the short distance expansion of the spectral representation of the scalar propagator in ϕ^4-theory and the quark propagator in QCD with their respective OPEs, constraints on both the spectral densities and the OPE condensates arise. On a qualitative level these constraints are interesting because they provide new information about the form of the spectral densities, and specifically the structure of the continuum contribution. In the case of QCD, this information can then be used to explicitly decompose the quark condensate $\langle \bar{\psi}\psi(0) \rangle$ into perturbative and non-perturbative contributions, and it turns out that the non-perturbative contributions are related to the structure of the continuum component of the scalar spectral density. More directly, these constraints may also provide useful information for procedures such as the SVZ sum rules which rely on constructing a parametrised form of the spectral density of certain correlation functions. A nice feature of this short distance matching approach is that it is completely model independent – it only relies on the existence of an OPE and a spectral representation. So in principle the analysis applied to the scalar and quark propagators in this paper can equally be applied to other interesting correlators such as the gluon propagator, the vector current correlator $\langle T \{ J_\mu(x) J_\nu(0) \} \rangle$, or other more general matrix elements, and this could potentially provide some interesting new insights.

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4.6 Appendix

It should be noted that in the short distance matching procedure carried out for the quark propagator, the calculations are implicitly performed in the Landau gauge[5]. In particular, the anomalous dimensions of the operators are calculated in this gauge [137]. In this sense the derived sum rules are gauge-dependent. However, this is not surprising since it is well-known that the renormalised quark (and gluon) spectral densities must depend explicitly on the gauge fixing parameter ξ [125]. This means that the sum rules derived for any of the propagators in QCD will therefore also depend on ξ. One could of course calculate the anomalous dimensions in an arbitrary ξ-gauge, and thus the sum rules would depend explicitly on ξ. Anomalous dimensions such as these have in fact already been calculated in the literature for certain fields in QCD [142]. However, the purpose of the work in Chap. 4 was to introduce a novel model-independent approach for determining non-perturbative information about spectral densities (and condensates), and to demonstrate the utility of this procedure.

As already alluded to in Chap. 4, the short distance matching procedure has many possible applications. One such application would be to probe the structure of hadronic correlators of the form $\langle T\{J_\mu(x)J_\nu(y)\}\rangle$. This could be done by starting with a parametrised hadronic ansatz for the spectral density, as in the SVZ approach, and then performing the short distance matching. In doing so this would automatically result in a series of relations between the hadronic and OPE parameters, one for each order in position which is matched. A nice feature of this approach is that these relations would be obtained without having to perform a Borel transformation, by contrast to the SVZ sum rules [119, 121]. Nevertheless, these ideas are beyond the scope of the investigations in Chap. 4, and so I leave them for future works.

[5] See [38, 39, 54] for more details about the Landau gauge and its properties.

Chapter 5

Conditions on the violation of the cluster decomposition property in QCD

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5.1 Abstract

The behaviour of correlators at large distances plays an important role in the dynamics of quantum field theories. In many instances, correlators satisfy the so-called *cluster decomposition property* (CDP), which means that they tend to zero for space-like asymptotic distances. However, under certain conditions it is possible for correlators to violate this property. In the context of quantum chromodynamics (QCD), a violation of the CDP for correlators of clusters involving coloured fields implies that the strength of the correlations between the coloured degrees of freedom in these clusters increases at large distances, which is a sufficient condition for confinement. In this paper we establish a criterion for when the CDP is violated. By applying this criterion to QCD, it turns out that certain lattice results involving the quark and gluon propagators can be interpreted as evidence that quarks and gluons are confined due to a violation of the CDP.

5.2 Introduction

Establishing the structure of correlators in a quantum field theory (QFT) is central to understanding the characteristics of the theory. In particular, the space-like asymptotic behaviour of truncated correlators comprised of field clusters determines how the strength of the correlations between the field degrees of freedom in these clusters changes as the distance between the clusters grows [77, 78]. This behaviour has been investigated several times in the literature[1], and a result of particular importance is the *cluster decomposition theorem* [77, 123]. This theorem characterises the asymptotic correlations between field clusters in QFTs which satisfy certain general axioms[2]. For QFTs which have a space of states with a positive-definite inner product, the cluster decomposition theorem implies that truncated correlators of field clusters tend to zero for large space-like distances [123], and in the case where the theory has a mass gap $(0, M)$, the rate of vanishing is faster than any inverse power of the distance. Correlators which have this behaviour are said to preserve the *cluster decomposition*

[1]See [123, 143–145] and references within.

[2]See [49–51] for a further discussion of these axioms and their physical motivation.

property (CDP). Physically, this means that the correlation strength between field clusters always decreases asymptotically if the corresponding correlator preserves the CDP. However, in the case of quantised gauge theories such as QCD, the standard QFT axioms no longer apply because locality is lost due to the gauge symmetry of the theory. Nevertheless, one can restore locality by adopting a *local quantisation*[3], which requires that the inner product in the space of states $\mathcal{V}$ is no longer positive-definite [47]. Having a space of states $\mathcal{V}$ with an indefinite inner product implies many consequences, including the modification of the cluster decomposition theorem. This modification has the particularly important feature that correlators are permitted to violate the CDP [77].

In the context of QCD, the modified cluster decomposition theorem has an important physical application – it provides a mechanism by which coloured degrees of freedom can be confined. Specifically, if the truncated correlator of coloured field clusters violates the CDP, then the correlations between the coloured degrees of freedom in these clusters are not damped, no matter how far they are separated. Thus, the measurement of a state associated with one of the coloured fields cannot be performed independently of the other, and hence the detection of individual coloured states is not possible, which is a sufficient condition for confinement [40, 51]. The failure of the CDP for such correlators is related to the inability to construct physical asymptotic states associated with the coloured fields [78]. Obtaining a better understanding of the general conditions under which the CDP is violated is therefore clearly important if one wants to establish whether QCD confinement occurs in this manner. It is these issues which we aim to shed light on in this paper.

The remainder of this paper is structured as follows: in Sec. 5.3 the cluster decomposition theorem is discussed, and conditions concerning the violation of the CDP are derived; in Sec. 5.4 the general Lorentz structure of QFT correlators is outlined and related to the CDP conditions in Sec. 5.3; in Sec. 5.5 the results of Secs. 5.3 and 5.4 are applied to QCD, and in particular specific lattice calculations involving the quark and gluon propagators; and finally in Sec. 5.6 the findings of the paper are summarised.

[3]One such example of this is the *BRST quantisation* of Yang-Mills theories [47].

5.3 The Cluster Decomposition Theorem

In locally quantised QFTs, a local field algebra is maintained at the expense of adding additional degrees of freedom to the theory, and results in a space of states $\mathcal{V}$ with an indefinite inner product [47]. The physical states $\mathcal{V}_{\text{phys}} \subset \mathcal{V}$ are subsequently characterised by a so-called *subsidiary condition*. For Yang-Mills gauge theories such as QCD, the most common local quantisation approach is *BRST quantisation*. In this case gauge fixing and ghost terms are added to the Lagrangian density, and the corresponding subsidiary condition is: $Q_B\mathcal{V}_{\text{phys}} = 0$, where Q_B is the conserved charge associated with the residual BRST symmetry which the modified Lagrangian density possesses. The Hilbert space is defined by $\mathcal{H} := \overline{\mathcal{V}_{\text{phys}}/\mathcal{V}_0}$, where $\mathcal{V}_0 \subset \mathcal{V}_{\text{phys}}$ contains the zero norm states, and the closure indicates that particular limit states are also in $\mathcal{H}$ [51]. As mentioned in Sec. 5.2, if a QFT has been locally quantised then the space-like asymptotic behaviour of cluster correlators is modified with respect to non-locally quantised theories. In particular, one has the following theorem [77]:

Theorem 5 (Cluster Decomposition)**.**

$$\left|\langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle^T\right| \leq \begin{cases} C_{1,2}[\xi]^{2N-\frac{3}{2}}e^{-M[\xi]}\left(1+\frac{|\xi_0|}{[\xi]}\right), & \textit{with a mass gap } (0,M) \textit{ in } \mathcal{V} \\ \widetilde{C}_{1,2}[\xi]^{2N-2}\left(1+\frac{|\xi_0|}{[\xi]^2}\right), & \textit{without a mass gap in } \mathcal{V} \end{cases}$$

where: $\langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle^T = \langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle - \langle 0|\mathcal{B}_1(x_1)|0\rangle\langle 0|\mathcal{B}_2(x_2)|0\rangle$, $N \in \mathbb{Z}_{\geq 0}$, $\xi = x_1 - x_2$ *is large and space-like, and* $C_{1,2}, \widetilde{C}_{1,2}$ *are constants independent of* ξ *and* N*.*

The *cluster correlator* $\langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle$ is defined by:

$$\begin{aligned}\langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle &:= \langle 0|\phi_1(f^{(1)}_{x_1})\phi_2(f^{(2)}_{x_2})|0\rangle \\ &= \int d^4y_1 d^4y_2\, \langle 0|\phi_1(y_1)\phi_2(y_2)|0\rangle f^{(1)}(y_1-x_1)f^{(2)}(y_2-x_2) \end{aligned} \tag{5.1}$$

where $f^{(i)} \in \mathcal{D}(\mathbb{R}^{1,3})$, and ϕ_k are the quantised *basic fields* in the theory[4]. The test functions $f^{(i)}$ are chosen to have compact support because this allows the operators

[4]The so-called *basic fields* [123, 143] consist of polynomials of the simplest fields, such as the quark ψ and gluon A^a_μ fields in QCD.

$\phi_1(f^{(1)}_{x_1})$ and $\phi_2(f^{(1)}_{x_2})$ to be interpreted as clusters containing the field degrees of freedom of ϕ_1 and ϕ_2, centred around the points x_1 and x_2 respectively. The precise definition of $[\xi]$ is outlined in [123], but for large space-like distances $[\xi]$ can be approximated by $|\boldsymbol{\xi}| := r$ [51]. It follows from Theorem 5 that in a locally quantised QFT such as QCD, if $\mathcal{V}$ does not have a mass gap, then the correlation strength $F^{\phi_1\phi_2}(r)$ between the clusters of the fields ϕ_1 and ϕ_2 has the asymptotic behaviour:

$$F^{\phi_1\phi_2}(r) \sim r^{2N-2}, \quad \text{for } r \to \infty \tag{5.2}$$

This has the important consequence that the CDP can be violated for $N \neq 0$, which as discussed in Sec. 5.2, is particularly relevant in the context of confinement in QCD.

In axiomatic formulations of QFT [49], the basic field correlators $\langle 0|\phi_1(y_1)\phi_2(y_2)|0\rangle = T_{(1,2)}(y_1 - y_2)$ are defined to be tempered distributions $\mathcal{S}'(\mathbb{R}^{1,3})$, and hence their Fourier transforms $\widehat{T}_{(1,2)}(p) = \mathcal{F}\left[T_{(1,2)}(y_1 - y_2)\right]$ are also in $\mathcal{S}'(\mathbb{R}^{1,3})$. Moreover, since

$$\langle 0|\mathcal{B}_1(x_1)\mathcal{B}_2(x_2)|0\rangle^T = \mathcal{T}^T_{(1,2)}(x_1 - x_2)$$

is the convolution of $\langle 0|\phi_1(y_1)\phi_2(y_2)|0\rangle^T = T^T_{(1,2)}(y_1 - y_2)$ with Schwartz test functions $f^{(i)} \in \mathcal{D}(\mathbb{R}^{1,3}) \subset \mathcal{S}(\mathbb{R}^{1,3})$, it follows that both $\mathcal{T}^T_{(1,2)}$ and its Fourier transform $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ are tempered distributions [61]. Due to the *spectral condition* axiom[5], $\widehat{T}^T_{(1,2)}(p)$ is also defined to have support in the closed forward light cone $\overline{V}^+$. By Eq. (5.1), $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ can be written:

$$\widehat{\mathcal{T}}^T_{(1,2)}(p) = \hat{f}^{(1)}(-p)\hat{f}^{(2)}(p)\widehat{T}^T_{(1,2)}(p) = g(p)\widehat{T}^T_{(1,2)}(p) \tag{5.3}$$

where $\hat{f}^{(i)} = \mathcal{F}\left[f^{(i)}\right] \in \mathcal{S}(\mathbb{R}^{1,3})$, and $g \in \mathcal{S}(\mathbb{R}^{1,3})$. So the convolution of $T^T_{(1,2)}$ with test functions in position space becomes a multiplication of $\widehat{T}^T_{(1,2)}$ with test functions in momentum space. Since $\operatorname{supp}\widehat{T}^T_{(1,2)} \subset \overline{V}^+$, Eq. (5.3) implies that $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ must also have support in $\overline{V}^+$. The parameter N in Theorem 5 depends on the structure of $\widehat{\mathcal{T}}^T_{(1,2)}(p)$. In particular, N is characterised by the following general theorem [146]:

Theorem 6 (Bros-Epstein-Glaser)**.** *Let $\mathscr{T} \in \mathcal{S}'(\mathbb{R}^{1,3})$ be a tempered distribution with support in $\overline{V}^+$. Then there exists a non-negative integer $N \in \mathbb{Z}_{\geq 0}$, and finite constant*

[5]The *spectral condition* axiom in QFT is related to the physical assumption that the energy spectrum of the theory is bounded from below [47].

$C > 0$, *such that:*

$$|\mathscr{T}(f)| \leq C \sum_{|\alpha|\leq N} \sup_{p\in\mathbb{R}^{1,3}} (1+\|p\|)^N |D^\alpha f(p)|, \quad \forall f \in \mathcal{S}(\mathbb{R}^{1,3})$$

where $\|p\|^2 = \sum_{\mu=0}^{3} |p_\mu|^2$, $D^\alpha = \frac{\partial^{|\alpha|}}{(\partial p_0)^{\alpha_0}\cdots(\partial p_3)^{\alpha_3}}$, *and:* $|\alpha| = \alpha_0+\alpha_1+\alpha_2+\alpha_3$

Theorem 6 is in fact a special case of the boundedness condition satisfied by all tempered distributions [61]. N corresponds to the highest number of derivatives $|\alpha|$ which appear in this bound. It is important to note though that N is not necessarily unique – a distribution may have different representations which each satisfy boundedness conditions with different numbers of derivatives. A more meaningful parameter is the *minimal* value of N over all possible representations, which is called the *order* of $\mathscr{T}$ [61]. In Theorem 5 one is interested in the *leading* asymptotic distance behaviour, and so N in this theorem corresponds to the order of $\widehat{\mathcal{T}}^{T}_{(1,2)}(p)$. To be consistent with Theorem 5, throughout the rest of this paper it will be implicitly assumed that N in Theorem 6 corresponds to the order of $\mathscr{T}$.

In light of Eq. (5.2), it is clearly important to establish whether one can determine a condition for when $N=0$. By applying Theorem 6, one in fact has the following necessary and sufficient condition:

Theorem 7. *Given that* $\mathscr{T} \in \mathcal{S}'(\mathbb{R}^{1,3})$ *has support in* $\overline{V}^+$

$$N = 0 \quad \Longleftrightarrow \quad \mathscr{T} \textit{ defines a finite measure}$$

Proof ($\Longrightarrow$)**:** Since $N=0$, from Theorem 6:

$$|\mathscr{T}(f)| \leq C \sup_{p\in\mathbb{R}^{1,3}} |f(p)|, \quad \forall f \in \mathcal{S}(\mathbb{R}^{1,3})$$

for some finite constant $C>0$. The linear functional $\mathscr{T}$ is therefore bounded, and hence continuous with respect to the topology induced by the norm $\|\cdot\|_\infty := \sup_{p\in\mathbb{R}^{1,3}}|\cdot|$. The restricted map $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ satisfies the same bound as $\mathscr{T}$ $\forall f \in C_c^\infty(\mathbb{R}^{1,3}) = \mathcal{S}(\mathbb{R}^{1,3}) \cap C_c^0(\mathbb{R}^{1,3})$, and since $C_c^\infty(\mathbb{R}^{1,3})$ with the norm $\|\cdot\|_\infty$ is a linear subspace of the normed vector space $(C_c^0(\mathbb{R}^{1,3}), \|\cdot\|_\infty)$, $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ is also linear. Conversely, if a linear map $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ satisfies a tempered distribution bound, then this same bound must *also* hold $\forall f \in \mathcal{S}(\mathbb{R}^{1,3})$, and so in this sense $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ (uniquely) defines $\mathscr{T}$ [61]. This means that one can think of $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ and $\mathscr{T}$ as corresponding to the *same* tempered distribution. As a consequence of the *Hahn-Banach Theorem* [147] it follows that $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ (and hence $\mathscr{T}$) can be extended to a linear functional $\widetilde{\mathscr{T}} : C_c^0(\mathbb{R}^{1,3}) \to \mathbb{C}$ which satisfies the same bound:

$$|\widetilde{\mathscr{T}}(g)| \leq C\|g\|_\infty, \quad \forall g \in C_c^0(\mathbb{R}^{1,3})$$

Moreover, due to this bound and the linearity of $\widetilde{\mathscr{T}}$ it follows that this extension is unique [62]. Since $\widetilde{\mathscr{T}}$ is a bounded linear functional on $C_c^0(\mathbb{R}^{1,3})$, the *Riesz Representation Theorem* [148] implies that there exists a unique finite (complex) regular Borel measure μ on $\mathbb{R}^{1,3}$ defined by:

$$\widetilde{\mathscr{T}}(g) = \int_{\mathbb{R}^{1,3}} g \; d\mu$$

In this sense $\widetilde{\mathscr{T}}$ is said to define a finite measure μ. Since $\widetilde{\mathscr{T}}$ is an unique extension which is entirely specified by $\mathscr{T}$, one defines $\widetilde{\mathscr{T}} \equiv \mathscr{T}$ with the understanding that when $\mathscr{T}$ acts on functions in $C_c^0(\mathbb{R}^{1,3})\backslash C_c^\infty(\mathbb{R}^{1,3})$, this is defined by the specific (unique) limit of $\mathscr{T}$ acting on a sequence of regularised test functions [62]. $\square$

Proof ($\Longleftarrow$)**:** Assuming μ is a finite measure implies [149] that $\mathscr{T}$ satisfies the bound:

$$|\mathscr{T}(g)| \leq \widetilde{C}\|g\|_\infty, \quad \forall g \in C_c^0(\mathbb{R}^{1,3})$$

for some finite $\widetilde{C} > 0$, and therefore the restricted map $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ also obeys this bound. From the discussion in the proof in the ($\Longrightarrow$) direction, $\mathscr{T}|_{C_c^\infty(\mathbb{R}^{1,3})}$ satisfying this bound is sufficient to imply that $\mathscr{T}$ must also have the same bound, but instead $\forall g \in \mathcal{S}(\mathbb{R}^{1,3})$. Since $|\mathscr{T}(g)| \leq \widetilde{C}\|g\|_\infty \, \forall g \in \mathcal{S}(\mathbb{R}^{1,3})$, it then follows from Theorem 6 that $N = 0$. $\square$

In the context of the cluster decomposition theorem (Theorem 5), Theorem 7 implies that $N = 0$ if and only if $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ defines a finite measure. So establishing whether $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ defines a finite measure or not is the key to determining how the correlation strength $F^{\phi_1\phi_2}(r)$ between the clusters of fields ϕ_1 and ϕ_2 changes as $r \to \infty$. Since $\widehat{\mathcal{T}}_{(1,2)}(p)$ satisfies Eq. (5.3), one has the following proposition:

Proposition 1. *If $\widehat{\mathcal{T}}^T_{(1,2)}$ defines a measure then this measure is finite.*

Proof. The condition for a tempered distribution to be finite as a measure is that the limit $\lim_{k\to\infty}|\widehat{\mathcal{T}}^T_{(1,2)}(\psi_k)|$ is finite, where $\psi_k \in \mathcal{D}(\mathbb{R}^{1,3})$ are a sequence of test functions such that $\lim_{k\to\infty}\psi_k = 1$. Computing this limit one has:

$$\lim_{k\to\infty}|\widehat{\mathcal{T}}^T_{(1,2)}(\psi_k)| = \lim_{k\to\infty}|g\widehat{T}^T_{(1,2)}(\psi_k)| = \lim_{k\to\infty}|\widehat{T}^T_{(1,2)}(g\psi_k)| = |\widehat{T}^T_{(1,2)}(g)| < \infty$$

where the final two identities follow from the continuity and boundedness of $\widehat{T}^T_{(1,2)}$ respectively. □

So in contrast to $\widehat{T}^T_{(1,2)}$, which can potentially define either a finite or an unbounded measure, measures defined by $\widehat{\mathcal{T}}^T_{(1,2)}$ can only be finite, independent of the form of the test functions $f^{(i)}$ used to define the clusters. Now if one combines Theorem 7 with Proposition 1, this implies the important corollary:

Corollary 5. *Given that $\widehat{\mathcal{T}}^T_{(1,2)} \in \mathcal{S}'(\mathbb{R}^{1,3})$ has support in $\overline{V}^+$, and is the Fourier transform of a truncated cluster correlator*

$$N = 0 \quad \Longleftrightarrow \quad \widehat{\mathcal{T}}^T_{(1,2)} \textit{ defines a measure}$$

Thus in order to determine if the Fourier transform of a such a cluster correlator has $N = 0$, one is only required to prove that the tempered distribution $\widehat{\mathcal{T}}^T_{(1,2)}$ defines a measure, since its finiteness is guaranteed. Conversely, if $\widehat{\mathcal{T}}^T_{(1,2)}$ can be shown to not define a measure, this is sufficient to prove that $N \neq 0$. A similar theorem was previously established by [78], in which the condition $N \neq 0$ is linked to the failure of Fourier transformed cluster correlators to define measures in some suitable neighbourhood of the light cone $\{p^2 = 0\}$. Corollary 5 is a generalisation of this theorem, since no restrictions are imposed on the neighbourhood in which $\widehat{\mathcal{T}}^T_{(1,2)}$ should fail to be a measure, only that it should fail to be a measure on $\mathbb{R}^{1,3}$. Moreover, the theorem by [78] implicitly assumes that $\mathcal{V}$ has no mass gap, whereas the proof of Theorem 7 (and hence Corollary 5) only depends on the support property of $\widehat{T}^T_{(1,2)}$.

When the structural form of correlators in QFTs are analysed and discussed, this is done almost exclusively with respect to the correlators involving the basic fields, and hence $\widehat{T}^T_{(1,2)}$. However, Corollary 5 emphasises that one can only determine if the CDP is violated or not if the structure of $\widehat{\mathcal{T}}^T_{(1,2)}$ is known. It is therefore important to establish what conditions $\widehat{\mathcal{T}}^T_{(1,2)}$ must satisfy in order to ensure that $\widehat{T}^T_{(1,2)}$ defines a measure, and vice versa. In this regard, one has the proposition:

Proposition 2. *If* $\widehat{T}^T_{(1,2)}$ *defines a measure* $\implies$ $\widehat{\mathcal{T}}^T_{(1,2)}$ *defines a measure*

Proof. $\widehat{\mathcal{T}}^T_{(1,2)}$ is a (linear) functional on $C^0_c(\mathbb{R}^{1,3})$ because: $\widehat{\mathcal{T}}^T_{(1,2)}(f) = g\widehat{T}^T_{(1,2)}(f) = \widehat{T}^T_{(1,2)}(gf)$ and $\widehat{T}^T_{(1,2)}$ is always well-defined on gf since $gf \in C^0_c(\mathbb{R}^{1,3})$ for $g \in \mathcal{S}(\mathbb{R}^{1,3})$ and $f \in C^0_c(\mathbb{R}^{1,3})$. Moreover, since g is bounded and $\widehat{T}^T_{(1,2)}$ defines a measure, it follows that for every compact set $K \subset \mathbb{R}^{1,3}$:

$$|\widehat{\mathcal{T}}^T_{(1,2)}(f)| = |\widehat{T}^T_{(1,2)}(gf)| \leq C_K \sup_{p\in K} |g(p)f(p)| \leq C_K \sup_{p\in K} |g(p)| \cdot \sup_{p\in K} |f(p)| \leq \widetilde{C}_K \sup_{p\in K} |f(p)|$$

holds for all f with support in K, and so $\widehat{\mathcal{T}}^T_{(1,2)}$ defines a measure. □

It is also clearly important to understand to what extent Proposition 2 holds in the opposite direction, or equivalently: what conditions must $\widehat{T}^T_{(1,2)}$ satisfy in order to ensure that $\widehat{\mathcal{T}}^T_{(1,2)}$ does not define a measure? One example of such a condition is summarised by the following proposition:

Proposition 3. *Let σ be a (tempered) distribution with discrete support, and $D\sigma$ the distributional derivative of σ.*

$$\widehat{T}^T_{(1,2)} = D\sigma \quad \implies \quad \widehat{\mathcal{T}}^T_{(1,2)} \textit{ does not define a measure}$$

Proof. In general, if σ has discrete support $\mathbb{S} \subset \mathbb{R}^{1,3}$, then $\sigma = \sum_{p\in\mathbb{S}} \sum_\alpha a_\alpha D^\alpha \delta_p$, where both sums are finite [61]. Assuming $f \in C^0_c(\mathbb{R}^{1,3})$, one has:

$$\begin{aligned}
\widehat{\mathcal{T}}^T_{(1,2)}(f) = g\widehat{T}^T_{(1,2)}(f) = \widehat{T}^T_{(1,2)}(gf) = D\sigma(gf) &= -\sigma(D(gf)) \\
&= -\sum_{p\in\mathbb{S}} \sum_\alpha a_\alpha D^\alpha \delta_p(D(gf)) \\
&= (-1)^{\alpha+1} \sum_{p\in\mathbb{S}} \sum_\alpha a_\alpha \delta_p \left[D^\alpha(fD(g) + gD(f))\right]
\end{aligned}$$

So the value of $\widehat{\mathcal{T}}^T_{(1,2)}(f)$ always depends on the derivative $D(f)$ evaluated at the points $p \in \mathbb{S}$. However, if f is not differentiable at some $p \in \mathbb{S}$, then $D(f)(p)$ is ill-defined, which proves that $\widehat{\mathcal{T}}^T_{(1,2)}$ cannot be a functional on $C^0_c(\mathbb{R}^{1,3})$, and therefore does not define a measure. $\square$

Together, Propositions 2 and 3 describe how the properties of $\widehat{T}^T_{(1,2)}(p)$ can be used to establish whether $\widehat{\mathcal{T}}^T_{(1,2)}(p)$ defines a measure, and thus by Corollary 5 whether N is vanishing or not. Since $\widehat{T}^T_{(1,2)}(p)$ is constructed purely in terms of the basic fields ϕ_k, the structure of $\widehat{T}^T_{(1,2)}(p)$ is constrained by Lorentz symmetry, which implies that $\widehat{T}^T_{(1,2)}(p)$ can be written in a general form. This form will be outlined in the next section, and its connection to the measure properties of $\widehat{T}^T_{(1,2)}(p)$ will be described.

5.4 The spectral structure of QFT correlators

5.4.1 The spectral representation

In axiomatic formulations of QFT, both $\widehat{T}^T_{(1,2)}(p)$ and $\widehat{T}_{(1,2)}(p)$ are *Lorentz covariant* tempered distributions, and therefore satisfy the following condition [56]:

$$\widehat{T}(\Lambda p) = S(\Lambda)\, \widehat{T}(p), \qquad \Lambda \in \overline{\mathscr{L}^{\uparrow}_{+}} \cong \mathrm{SL}(2,\mathbb{C}) \tag{5.4}$$

where $\overline{\mathscr{L}^{\uparrow}_{+}}$ is the universal cover of the identity component of the Lorentz group[6] $\mathscr{L}^{\uparrow}_{+}$, and S is some (finite-dimensional) representation of $\mathrm{SL}(2,\mathbb{C})$. In the special case where the representation is trivial ($S(\Lambda) \equiv 1$), $\widehat{T}(p)$ is called a *Lorentz invariant* distribution. The structure of the Lorentz covariant distribution $\widehat{T}(p)$ is dependent upon how the fields ϕ_1 and ϕ_2 transform under Lorentz transformations. In particular, $\widehat{T}(p)$ has the following decomposition [56]:

$$\widehat{T}(p) = \sum_{\alpha=1}^{\mathscr{N}} Q_\alpha(p)\, \widehat{T}_\alpha(p) \tag{5.5}$$

[6]This group consists of Lorentz transformations that preserve both orientation and the direction of time.

where $\widehat{T}_\alpha(p)$ are Lorentz invariant distributions, and $Q_\alpha(p)$ are Lorentz covariant polynomial functions of p which carry the Lorentz index structure of ϕ_1 and ϕ_2. The simplest case is the Fourier transform of a correlator involving two scalar fields. Since both the fields are scalar it follows that $Q_1(p) = 1$, and therefore $\widehat{T}(p) = \widehat{T}_1(p)$. As an example, consider $\widehat{D}(p) = \mathcal{F}\left[\langle 0|\phi(x)\phi(y)|0\rangle\right]$, where ϕ is a free scalar field of mass m. In this case $\widehat{D}(p)$ has the explicit form:

$$\widehat{D}(p) = a\,\delta(p) + 2\pi\theta(p^0)\delta(p^2 - m^2) \tag{5.6}$$

where $a = |\langle 0|\phi|0\rangle|^2$, and hence: $\widehat{D^T}(p) = 2\pi\theta(p^0)\delta(p^2 - m^2)$. The truncation of the scalar correlator therefore removes the component of $\widehat{D}(p)$ concentrated at $p = 0$. As expected from Eq. (5.5), the overall structure of $\widehat{D}(p) = \widehat{D}_1(p)$ (and also $\widehat{D^T}(p)$) is Lorentz invariant.

Now consider the case where $\widehat{S}(p)$ is the Fourier transform of a correlator that involves a Dirac spinor and conjugate spinor field. Here there exist two possible Lorentz covariant polynomials: $Q_1(p) = \mathbb{I}$ and $Q_2(p) = \gamma^\mu p_\mu = \not{p}$, and hence:

$$\widehat{S}(p) = \mathbb{I}\,\widehat{S}_1(p) + \not{p}\,\widehat{S}_2(p) \tag{5.7}$$

where the spinor indices have been suppressed. In the case where $\widehat{S}(p) = \mathcal{F}\left[\langle 0|\psi(x)\overline{\psi}(y)|0\rangle\right]$, and ψ is a free Dirac field of mass m, $\widehat{S}(p)$ has the explicit form:

$$\widehat{S}(p) = 2\pi(\not{p} + m)\theta(p^0)\delta(p^2 - m^2) \tag{5.8}$$

Comparing this expression with Eq. (5.7) it follows that $\widehat{S}_1(p) = 2\pi m\,\theta(p^0)\delta(p^2 - m^2)$, and $\widehat{S}_2(p) = 2\pi\theta(p^0)\delta(p^2 - m^2)$, which again as anticipated are both Lorentz invariant. Finally, consider a Fourier transformed correlator $\widehat{D}_{\mu\nu}(p)$ that involves two arbitrary vector fields with indices μ and ν respectively. In this case there are also two possible Lorentz covariant polynomials: $Q_1(p) = g_{\mu\nu}$ and $Q_2(p) = p_\mu p_\nu$, which implies:

$$\widehat{D}_{\mu\nu}(p) = g_{\mu\nu}\,\widehat{D}_1(p) + p_\mu p_\nu\,\widehat{D}_2(p) \tag{5.9}$$

An example of this class of Lorentz covariant distributions is: $\widehat{D}_{\mu\nu}(p) = \mathcal{F}\left[\langle 0|A_\mu(x)A_\nu(y)|0\rangle\right]$, where A_μ is a free (abelian) gauge field. One can demonstrate that $\widehat{D}_{\mu\nu}(p)$ has the form [56]:

$$\widehat{D}_{\mu\nu}(p) = 2\pi\theta(p^0)\left[-g_{\mu\nu}\delta(p^2) + (\xi - 1)\delta'(p^2)p_\mu p_\nu\right] \tag{5.10}$$

where ξ is the gauge-fixing parameter which is introduced in order to locally quantise the theory. Comparing this expression with Eq. (5.9), $\widehat{D_1}(p) = -2\pi\theta(p^0)\delta(p^2)$ and $\widehat{D_2}(p) = 2\pi\theta(p^0)(\xi-1)\delta'(p^2)$, which are both Lorentz invariant.

Now that the general structure of Lorentz covariant (Fourier transformed) correlators in QFTs has been outlined, the results of Sec. 5.3 can be applied to some explicit physical examples. Firstly, consider the free quantised electromagnetic field A_μ. The Fourier transform of the correlator of this field is given by Eq. (5.10). The non-gauge-fixing component of $\widehat{D}_{\mu\nu}(p)$ clearly defines a measure, whereas for general values of ξ, the gauge-fixing component contains a $\delta'(p^2)$ term, which does not define a measure. However, since the physical characteristics of gauge theories are independent of the value of the ξ, one is free to set $\xi = 1$, and then $\widehat{D}_{\mu\nu}(p) = -2\pi g_{\mu\nu}\theta(p^0)\delta(p^2)$. Since[7] $\langle 0|A_\mu(x)A_\nu(y)|0\rangle^T = \langle 0|A_\mu(x)A_\nu(y)|0\rangle$, and $\widehat{D}^T_{\mu\nu}(p) = \widehat{D}_{\mu\nu}(p)$ defines a measure, it follows from Proposition 2 and Corollary 5 that the CDP is preserved ($N = 0$). Due to Theorem 5, physically this implies that the correlation strength $F^{\gamma\gamma}_{\text{free}}(r)$ between clusters containing free photons has the asymptotic behaviour:

$$F^{\gamma\gamma}_{\text{free}}(r) \sim \frac{1}{r^2}, \qquad r \to \infty \tag{5.11}$$

and hence the correlation between free photons becomes increasingly weaker the further away they are separated.

In QCD, the correlators of interest involve quark and gluon fields. Unlike the photon field, the non-abelian gluon field A^a_μ can never be free because there are always (self) interactions, even with the absence of quark fields. It is possible though to consider free quarks, and in fact the Fourier transformed free quark correlator $\widehat{S}(p)$ has the form of Eq. (5.8), where now m is the mass of the quark. Because[8] $\langle 0|\psi(x)\overline{\psi}(y)|0\rangle^T = \langle 0|\psi(x)\overline{\psi}(y)|0\rangle$, and $\widehat{S}^T(p) = \widehat{S}(p)$ defines a measure, Proposition 2 and Corollary 5 imply that $N = 0$. Since the theory contains a mass gap $(0, m)$, it follows from Theorem 5 that the correlation strength $F^{q\bar{q}}_{\text{free}}(r)$ between free quarks behaves asymptotically as:

$$F^{q\bar{q}}_{\text{free}}(r) \sim \frac{e^{-mr}}{r^{\frac{3}{2}}}, \qquad r \to \infty \tag{5.12}$$

[7] The equality $\langle 0|A_\mu(x)A_\nu(y)|0\rangle^T = \langle 0|A_\mu(x)A_\nu(y)|0\rangle$ follows from Lorentz invariance [47].

[8] $\langle 0|\psi(x)\overline{\psi}(y)|0\rangle^T = \langle 0|\psi(x)\overline{\psi}(y)|0\rangle$ also because of Lorentz invariance.

and hence free quarks preserve the CDP. Physically, this means that the correlation between the quarks is exponentially suppressed at large distances, which supports the hypothesis that free quarks are not confined, as one would expect.

Although the examples considered so far have consisted of exactly solvable free theories, the results derived in Sec. 5.3 are also equally applicable to interacting QFTs. However, in general the analytic structure of correlators is poorly understood for interacting theories, and so it is more difficult to prove directly whether the CDP is preserved or not. Quantum electrodynamics (QED) is one example of an interacting theory though, where it is possible to determine this property [51]. In QED, $F_{\mu\nu}$ is an observable, which implies that $\langle 0|F_{\mu\nu}(x)F_{\rho\sigma}(y)|0\rangle$ is a positive-definite distribution[9] [51]. Positive-definiteness is sufficient to prove that $\mathcal{F}\left[\langle 0|A_\mu(x)A_\nu(y)|0\rangle^T\right]$ is non-negative, defines a measure [56], and thus by Proposition 2 $N=0$, which implies that interacting photons also preserve the CDP. In QCD though, this same argument fails because $F^a_{\mu\nu}$ is *not* an observable, which itself is a consequence of the non-abelian nature of the theory. The failure of this proof is certainly suggestive that the CDP may no longer hold for the gluon cluster correlator in QCD. However, as emphasised by [40], the failure of this proof is not same as a proof of its failure, and it remains an open question as to whether the gluon correlator, or more generally cluster correlators of coloured fields, violate the CDP. The problem in QCD is that the precise form of correlators involving coloured fields is controlled by the non-perturbative dynamics of the theory, which is *a priori* unknown. Nevertheless, the general non-perturbative structure of these correlators can still be characterised in a general manner, and this will be discussed in the following section.

5.4.2 The spectral density

Due to Eq. (5.5), it is clear that in order to characterise Fourier transformed correlators, it is important to understand the general structure of Lorentz invariant distributions $\widehat{T}_\alpha$. As discussed in Sec. 5.3, these distributions are also required to have support in the closed forward light cone $\overline{V}^+$. If a tempered distribution $\widehat{T}_\alpha \in \mathcal{S}'(\mathbb{R}^{1,3})$ is both

[9] A positive-definite distribution $T(x-y)$ satisfies the condition: $\int d^4x d^4y\, T(x-y)\overline{f(x)}f(y) \geq 0$ for any test function f.

Lorentz invariant, and has support in $\overline{V}^{+}$, it turns out that $\widehat{T}_{\alpha}$ can be written in the following general manner [56]:

$$\widehat{T}_{\alpha}(p) = P(\partial^2)\delta(p) + \int_0^{\infty} ds\, \theta(p^0)\delta(p^2 - s)\rho_{\alpha}(s) \tag{5.13}$$

where $P(\partial^2)$ is some polynomial in the d'Alembert operator $\partial^2 = g_{\mu\nu}\frac{\partial}{\partial p_{\mu}}\frac{\partial}{\partial p_{\nu}}$, and $\rho_{\alpha}(s) \in \mathcal{S}'(\bar{\mathbb{R}}_{+})$. This important structural relation is called the *spectral representation* of $\widehat{T}_{\alpha}$, and ρ_{α} is referred to as the *spectral density*. If $\widehat{T}_{\alpha}$ is also a non-negative distribution[10], it follows that $\widehat{T}_{\alpha}(f) = \int f(p)\, d\mu(p)$, where $d\mu(p)$ is a non-negative (tempered) measure. In this case $\widehat{T}_{\alpha}(p)$ has the form:

$$\widehat{T}_{\alpha}(p) = c\,\delta(p) + \int_0^{\infty} ds\, \theta(p^0)\delta(p^2 - s)\rho_{\alpha}(s) \tag{5.14}$$

where $c \geq 0$, and $\rho_{\alpha}(s)$ defines a (tempered) measure $d\rho_{\alpha}(s) = \rho_{\alpha}(s)ds$. Eq. (5.14) is called the *Källén-Lehmann representation*. In fact, independently of whether $\widehat{T}_{\alpha}$ is non-negative or not, if $\widehat{T}_{\alpha}$ defines a measure then this is sufficient to imply that $\widehat{T}_{\alpha}$ must have the form of Eq. (5.14), but c is not necessarily positive in this case.

The spectral representation of $\widehat{T}_{\alpha}$ emphasises that the $\mathscr{N}$ spectral densities ρ_{α} associated with a correlator play a fundamental role in determining its structure. In fact, when $\widehat{T}_{\alpha}$ is a measure, and Eq. (5.14) holds, correlators are uniquely specified by $\{\rho_{\alpha}\}$. Comparing the Fourier transformed free correlator components $\widehat{S}_{i}(p)$ and $\widehat{D}_{i}(p)$ discussed in Sec. 5.4.1 with Eq. (5.13), one can directly see that the spectral densities for the Dirac correlator are:

$$\rho_1^{\psi}(s) = 2\pi m\, \delta(s - m^2), \qquad \rho_2^{\psi}(s) = 2\pi\delta(s - m^2) \tag{5.15}$$

and for the vector field correlator are:

$$\rho_1^{A}(s) = -2\pi\delta(s), \qquad \rho_2^{A}(s) = 2\pi(\xi - 1)\delta'(s) \tag{5.16}$$

In Eq. (5.15), both of the spectral densities define measures. This is not surprising because $\widehat{S}(p)$ itself defines a measure, and therefore both $\widehat{S}_1(p)$ and $\widehat{S}_2(p)$ must satisfy Eq. (5.14). In Eq. (5.16) though, ρ_1^{A} defines a measure but ρ_2^{A} clearly does not, unless $\xi = 1$. That ρ_2^{A} is permitted to not define a measure is a symptom of the fact that

[10] A non-negative distribution $\widehat{T}_{\alpha}$ has the property that $\widehat{T}_{\alpha}(f) \geq 0$, $\forall f \geq 0$.

much like QCD, a free quantised abelian gauge theory is a locally quantised QFT. As discussed in Sec. 5.2, this means that the space of states $\mathcal{V}$ no longer has a positive-definite inner product. This implies, among other things, that the Fourier transformed correlators are not guaranteed to be non-negative, and so may not define measures and satisfy Eq. (5.14) [56].

It is clear from the results in this section that the behaviour of correlators is closely connected to the structure of the associated spectral densities $\{\rho_\alpha\}$. In light of Eqs. (5.5) and (5.14) it is clear that if any of the spectral densities ρ_α does not define a measure, then this is sufficient to imply that $\widehat{T}$ must also not define a measure. However, as already mentioned in Sec. 5.3, the failure of $\widehat{T}^T_{(1,2)}$ to define a measure may not imply that $\widehat{\mathcal{T}}^T_{(1,2)}$ does not define a measure, and that $N \neq 0$. But by Proposition 3, if $\widehat{T}^T_{(1,2)} = D\sigma$ where σ is a distribution with discrete support, then this *is* sufficient to imply that $N \neq 0$. In fact, if any of the components in the Lorentz covariant decomposition of $\widehat{T}^T_{(1,2)}$ contains a term of the form $D\sigma$, then this implies that $N \neq 0$. The simplest such example is if $\widehat{T}^T_{(1,2)}(p) = \theta(p^0)\delta'(p^2 - a)$, and hence by Eq. (5.13), $\rho(s) = \delta'_a(s) = \delta'(s-a)$, as is the case for ρ_2^A in Eq. (5.16) (with $\xi \neq 1$ and $a = 0$). Therefore, if the spectral densities of any (truncated) correlator contain a δ'_a term, this is sufficient to imply that $N \neq 0$. This result is particularly interesting when applied to QCD because it provides a definite condition with which to test whether truncated cluster correlators of coloured fields violate the CDP. Both this condition and its applications will be discussed in the next section.

5.5 The cluster decomposition property in QCD

As outlined at the end of the Sec. 5.4.2, determining the structure of the spectral densities of correlators that involve coloured fields in QCD, such as the quark and gluon correlators, is a direct way to establish whether $N = 0$ or not. In particular, if any of the spectral densities contain a δ'_a term, this is sufficient to imply that $N \neq 0$. Combining this result with Theorem 5, one has the following corollary:

Corollary 6. *Assuming that the state space $\mathcal{V}_{QCD}$ has no mass gap, and that any of the spectral densities $\{\rho_\alpha\}$ of correlators involving coloured fields contains a δ'_a term,* *this is sufficient to ensure confinement.*

It is important to emphasise here that the requirement of no mass gap refers to the full state space $\mathcal{V}$ (with an indefinite inner product), and not to the physical Hilbert space $\mathcal{H}$. In particular, this means that it is possible for $\mathcal{V}$ to have no mass gap but $\mathcal{H}$ to have one, which is expected to be the case in QCD [51]. Since the precise analytic form of spectral densities (and hence correlators) are unknown in QCD, it is difficult to establish whether $\{\rho_\alpha\}$ contain non-measure defining terms or not. Nevertheless, by using non-perturbative methods such as lattice QFT it is possible to calculate approximations to these objects using numerical fits. An important expression in this regard is the so-called *Schwinger function* $C_\alpha(t)$, which can be written in the following form[11]:

$$C_\alpha(t) = \int_0^\infty ds\, \rho_\alpha(s) \frac{e^{-\sqrt{s}\,t}}{2\sqrt{s}} \tag{5.17}$$

where ρ_α is the spectral density associated with one of the components of a specific propagator[12], and $t \geq 0$. By calculating $C_\alpha(t)$ on the lattice, this provides a way of indirectly probing the structure of ρ_α. $C_\alpha(t)$ has been computed for both the quark and gluon propagators, and one of the most striking features is that $C_\alpha(t)$ appears to become negative at some value of t [126, 127]. This feature implies that ρ_α violates non-negativity, which is usually interpreted as evidence of confinement [126, 127]. However, it is often assumed that $\rho_\alpha(s)$ makes sense as a function, and that the negativity of $C_\alpha(t)$ is due to $\rho_\alpha(s)$ becoming negative over some continuous range of s [150]. In general though, because ρ_α is a distribution (in $\mathcal{S}'(\bar{\mathbb{R}}_+)$), ρ_α could equally contain both regular and singular components, and so the negativity of $C_\alpha(t)$ is not necessarily caused by $\rho_\alpha(s)$ becoming negative as a continuous function. In fact, by inserting a singular term of the form $B\delta_b'$ into Eq. (5.17) (with $b > 0$ and $B < 0$), it is clear that the appearance of such a term can cause $C_\alpha(t)$ to become continuously negative. Moreover, the shape characteristics of $C_\alpha(t)$ can also be replicated. Lattice calculations

[11] In general, the Schwinger function is defined by: $C_\alpha(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dp_0\, e^{ip_0 t}\Delta_\alpha(p^2)|_{\mathbf{p}=0}$, where $\Delta_\alpha(p^2)$ is one of the components of a Euclidean propagator. It should be noted that $C_\alpha(t)$ reduces to the form of Eq. (5.17) only if one assumes that $\Delta_\alpha(p^2)$ does not contain $P(\partial^2)\delta(p)$ contributions as in Eq. (5.13).

[12] The spectral densities $\{\rho_\alpha\}$ which define correlators are the same as those that define propagators. Moreover, $\{\rho_\alpha\}$ have the same form for both Euclidean and Minkowski spacetime propagators.

of both the quark and gluon propagators indicate that $C_\alpha(t)$ starts positive for small t, becomes negative at some specific value of t, and then generally flattens towards zero for large values of t. By employing a spectral density ansatz of the form: $\rho_\alpha(s) = A\delta(s-a) + B\delta'(s-b)$, where $A > 0$ and $B < 0$ ($a, b > 0$ by definition), this qualitative behaviour is reproduced. This specific example demonstrates that the spectral density ρ_α can in fact be completely singular, and yet still reproduce the observed behaviour of $C_\alpha(t)$. In light of Corollary 6, the characteristics of $C_\alpha(t)$ can therefore instead be interpreted as evidence of confinement caused by the failure of the CDP for quarks and gluons.

In some cases, the spectral densities of propagators (and hence correlators) are explicitly computed using a combination of numerical and analytic approaches[13]. This then means that the explicit form of $\widehat{\mathcal{T}}^{T}_{(1,2)}$ can be determined using Eq. (5.13), and thus Corollary 5 can actually be applied directly to determine whether $N = 0$ or not. Of course, if one can demonstrate that $N \neq 0$, it is also interesting to establish the specific value that N takes, especially in the case of the quark and gluon correlators where N determines how the correlation strength $F(r)$ between the quark and gluon field clusters behaves as $r \to \infty$. However, as discussed in Sec. 5.3, if one constructs a bound on $\widehat{\mathcal{T}}^{T}_{(1,2)}$ (as in Theorem 6), one is not guaranteed that the largest value of $|\alpha|$ which appears in this bound is minimal. If the maximal value of $|\alpha|$ equals m say, then one can only assert that the order of $\widehat{\mathcal{T}}^{T}_{(1,2)}$ satisfies: $N \leq m$. Nevertheless, this is still interesting because it implies an upper bound on the asymptotic behaviour of $F^{q\bar{q}}(r)$ and $F^{gg}(r)$.

The discussions in this section demonstrate that confinement may occur in QCD because of a violation of the CDP caused by the appearance of non-measure defining δ'_a terms in the spectral densities of coloured correlators. In particular, the negativity of $C_\alpha(t)$ for quark and gluon propagators can be interpreted as evidence of such a violation, and therefore supports the hypothesis of quark and gluon confinement. Due to Theorem 5 and Corollary 5, whether a truncated cluster correlator violates the CDP or not depends on if its Fourier transform defines a measure, which itself is determined by the structure of the corresponding spectral densities $\{\rho_\alpha\}$. Although we will not pursue this further here, it would be interesting to establish whether the constraints

[13] See for example [151] and [135].

imposed on $\{\rho_\alpha\}$ by the requirement to preserve or violate the CDP are consistent with the constraints due to other physical or structural relations, such as the operator product expansion [2].

5.6 Conclusions

Determining the space-like asymptotic behaviour of truncated cluster correlators is crucial for understanding the large-distance correlation strength between the effective quanta associated with the field degrees of freedom in these correlators. For a QFT which is locally quantised, the cluster decomposition theorem implies that it is possible for a truncated cluster correlator to grow asymptotically, and hence violate the CDP, provided that the order of the correlator N is non-vanishing. This possibility is particularly interesting in the context of QCD, as it provides a mechanism for which coloured degrees of freedom, such as quarks and gluons, can become confined. In this paper, we established a necessary and sufficient condition for a truncated cluster correlator to have $N = 0$. It turns out that whether N vanishes or not depends entirely on if the Fourier transform of the correlator defines a measure, which itself is determined by the structure of the spectral densities $\{\rho_\alpha\}$ of the correlator. Applying these results to QCD, it follows that if the indefinite inner product state space $\mathcal{V}_{\mathrm{QCD}}$ has no mass gap, and any of the spectral densities of correlators involving coloured fields contains a δ'_a term, then this is sufficient to ensure confinement. In this context, the negativity of the Schwinger functions $C_\alpha(t)$ for the quark and gluon propagators on the lattice can therefore be interpreted as evidence that quarks and gluons are confined because they violate the CDP.

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5.7 Appendix

As discussed in Sec. 5.5, lattice calculations of the Schwinger function $C_\alpha(t)$ provide a way of probing the structure of the spectral densities ρ_α of the QCD propagators. Of course, the lattice techniques for calculating $C_\alpha(t)$, namely the Dyson-Schwinger equations, carry inherent theoretical and computational uncertainties[14]. Nevertheless, $C_\alpha(t)$ has been calculated numerous times by different collaborations, with all of the results confirming that $C_\alpha(t)$ becomes negative at some value of t for both the quark and gluon propagators [150]. The qualitative fact that $C_\alpha(t)$ appears to become negative is actually sufficient to suggest that the spectral density may contain a non-measure defining δ'_a component. In other words, the precise quantitative behaviour of $C_\alpha(t)$ is not required in order to make this statement. It should also be noted here that lattice studies never actually measure the spectral densities ρ_α directly, only some smeared version (in this case $C_\alpha(t)$). So even though ρ_α are distributions, the (possibly singular) behaviour of ρ_α can still be probed. This is discussed for example in [126] and [124], where it is pointed out that if ρ_α contains a δ singularity, then lattice calculations of $C_\alpha(t)$ would find that it has an exponentially decreasing behaviour, but is non-negative.

[14]See [125] for a more detailed discussion of these issues.

Chapter 6

Summary and Outlook

The main conclusions from each chapter are outlined in Secs. 2.6, 4.5, 3.5 and 5.6. In this section the key results will be summarised, and an overview given. The main theme of Chap. 2 is that spatial boundary operators play an important role in QFTs, especially with regards to the so-called *proton spin crisis*, which concerns the question of whether the angular momentum operator in QCD J_{QCD} possesses a meaningful quark-gluon decomposition. It turns out that there are many different possible decompositions of J_{QCD}, and that for them to hold it is necessary that specific spatial boundary operators vanish. An AQFT approach is subsequently used to derive a condition for when spatial boundary operators vanish, and somewhat surprisingly it transpires that if the operator annihilates the vacuum state, this is both necessary and sufficient to ensure that the operator vanishes, independently of how it acts on the full space of states. By applying this condition to the corresponding spatial boundary operator that appears in the Jaffe-Manohar decomposition, one of the original decompositions proposed in the literature, it follows that this operator is non-vanishing precisely because of the non-vanishing of certain QCD condensates. Since the structure of these condensates is determined by the non-trivial (non-perturbative) vacuum structure of QCD, this leads to the physical conclusion that forming distinct quark and gluon spin observables in this manner is prevented precisely because of the breakdown of the particle interpretation for quarks and gluons in QCD.

Similarly with Chap. 2, Chap. 3 investigates the role of spatial boundary operators in QFT, but instead in the context of non-manifest symmetries and their quantisation. An important characteristic of this class of symmetries is that the conserved currents associated with these symmetries are only defined up to the addition of an anti-symmetric improvement term. The corresponding charges associated with these different currents must therefore differ by a spatial boundary operator. From the results in Chap. 2 it follows that spatial boundary operators are not guaranteed to vanish, and so the charge operator is therefore not uniquely defined. Nevertheless, it follows that different expressions for the charge operator are all still guaranteed to generate *the same* symmetry transformation. An immediate consequence of this is that despite the non-uniqueness of the charge, the criterion for the symmetry to be spontaneously broken is unaffected by this property. However, the non-uniqueness of the charge implies that the action of the charge operator on states is potentially ambiguous. In the latter part of Chap. 3, these results are applied to specific examples of non-manifest symmetries: translational invariance, Lorentz invariance, and supersymmetry. In the case of the first two symmetries, the physical assumption (Axiom 3) that the vacuum is the unique translational (and hence Poincaré) invariant state is sufficient to uniquely specific the charges associated with these symmetries. However, for supersymmetry there is no equivalent physical requirement, and hence the supersymmetric charge is not uniquely defined. The findings in this chapter illustrate an important point; classical and quantised field theories can often differ significantly in their structure, and thus classical reasoning is not necessarily valid for QFTs.

In Chap. 4, the main focus was the development of a novel method to determine information about the spectral densities of propagators in QFTs. Specifically, this approach consists of matching the x-coefficients in the short distance expansion of the spectral representation of a propagator, with its corresponding OPE. For each order of x considered in the expansions, one obtains a constraint on a specific moment of a spectral density. In order to explicitly demonstrate the utility of this method, the procedure is applied to the scalar propagator in ϕ^4-theory and the quark propagator in QCD. It turns out in both of these cases that not only does one constrain the explicit form of the corresponding spectral densities, but that these constraints enable the condensates that appear in the OPE to be decomposed into perturbative and non-perturbative components, a feature which has previously only been assumed, but never explicitly derived before in the literature. In the case of the quark propagator, an explicit decomposition of the quark condensate $\langle\overline{\psi}\psi\rangle$ is derived. Interestingly, the non-perturbative contribution to this condensate is shown to be related to the structure of the continuum component of the scalar spectral density. A particularly nice feature of this short distance matching method is that it is completely model independent – it only relies on the existence of an OPE and a spectral representation. Although this method was applied only to the scalar and quark propagators in Chap. 4, it can equally be applied to any other correlation function, and therefore has many potential applications.

Finally, in Chap. 5 the large-distance properties of correlation functions is investigated. An important result in this regard is the *cluster decomposition theorem*, which specifies how truncated cluster correlators behave as the (space-like) distance between the clusters becomes asymptotic. This behaviour corresponds to the large-distance correlation strength between the field degrees of freedom in these clusters. An intriguing feature of locally quantised QFTs, such as BRST quantised QCD, is that the cluster decomposition theorem permits truncated cluster correlators to *grow* asymptotically (violate the CDP), provided that the (indefinite inner product) state space $\mathcal{V}$ has no mass gap, and the order of the correlator N is non-zero. This feature is particularly relevant for QCD, since it illustrates the possibility that the correlation strength between clusters containing coloured degrees of freedom could *increase* as the clusters are moved further apart, which is a sufficient condition for confinement. Therefore, to establish whether this mechanism occurs or not in QCD, it is clearly important to determine a criterion for when N vanishes. It turns out in fact that there exists both a necessary and sufficient condition for when $N = 0$, and this is derived in Chap. 5. This condition states that $N = 0$ if and only if the Fourier transform of the correlator defines a measure, which itself it related to the structure of the spectral densities associated with this correlator. In QCD, the behaviour of spectral densities can be analysed by performing calculations on the lattice. At the end of Chap. 5 it is demonstrated that the properties of certain lattice calculations involving the quark and gluon propagators can be interpreted as evidence that the spectral densities contain a δ'_a component. If one assumes that $\mathcal{V}_{\mathrm{QCD}}$ has no mass gap, then this suggests that both quarks and gluons are confined due to a violation of the CDP. In principle, the results derived in Chap. 5 could also equally be used to analyse the structure of coloured correlators. It would also be interesting to explore the connection between the spectral density constraints derived in Chap. 4 and the conclusions drawn in this chapter.

The investigations performed throughout the chapters of this thesis cover a broad range of different topics in particle physics. Since axiomatic QFT has been an integral component in each of these investigations, this clearly demonstrates both the utility and scope of this approach. It is clear that the performance of perturbative and phenomenological calculations is still essential if one wants to understand experimental results, but these approaches alone are not capable of fully describing these results, since their consistency is not guaranteed for all kinematic regimes. AQFT though is by construction always well-defined, and so provides a powerful framework from which these methods can be rigorously understood. Moreover, this framework enables one to analyse non-perturbative phenomena in a consistent manner, and ultimately has the potential to make profound non-perturbative predictions. A particularly important feature of this approach is that the foundations are based on a series of physically motivated axioms, and hence the assumptions behind predictions are clear from the outset. Therefore, if a prediction does not agree with experimental evidence, this implies that one (or more) of the foundational axioms is not physically reasonable, and hence must be modified. Despite the consistency and success of this procedure, the pursuit to fully axiomatise realistic QFTs in 1+3 dimensions is a seemingly difficult problem, which has not yet yielded a solution. Nevertheless, the analysis performed in Chaps. 2–5 of this thesis demonstrates that a lot of insightful information about physically relevant theories can be obtained by using this approach without having to solve the full theory.

The field of particle physics is currently in a state of flux; most experimental evidence confirms the SM to a high precision, and there is no distinguished model that seems to unambiguously describe the observed deviations. Moreover, the SM itself contains phenomena such as QCD confinement and hadronisation which still remain poorly understood. It is for these reasons that I believe that now it is more important then ever to utilise and develop axiomatic QFT approaches. Over the last few decades, AQFT has consistently demonstrated an effectiveness in shedding new light on problems in QFT, and making deep predictions which are consistent with experiment. Nevertheless, AQFT is rarely discussed in the literature, especially in the context of either the SM or BSM theories. Therefore, in order to better understand in which theoretical direction particle physics should proceed, it is essential that the ideas of AQFT are taken into account in this pursuit.

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Publications

- ◇ P. Lowdon, "Conditions on the violation of the cluster decomposition property in QCD," (2015) [arXiv:1511.02780] (Accepted for publication in *J. Math. Phys.*).
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Seminars and Talks

◇ Zurich Physics PhD Seminar, "Boundary terms in the decomposition of nucleon spin," Paul Scherrer Institute, 27th August 2015.

◇ XXIII International Workshop on Deep-Inelastic Scattering 2015, "Boundary terms in the decomposition of nucleon spin," Southern Methodist University, 28th April 2015.

◇ Sinergia Meeting, "The proton spin crisis and form factors," University of Bern, 9th September 2014.

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